A THREE-DIMENSIONAL FINITE DIFFERENCE TIME DOMAIN - PERFECTLY MATCHED LAYER ALGORITHM FOR NONLINEAR DISPERSIVE MEDIA

S. Joe Yakura

10 March 2000

Final Report

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A Three-Dimensional FDTD-PML Algorithm for Nonlinear Dispersive Media

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Abstract

Starting with the unsplit-field uniaxial PML formulation, a second-order accurate FDTD-PML algorithm is obtained for the first time using the piecewise-linear approximation for nonlinear dispersive PML media. In the absence of the PML interface, the nonlinear dispersive FDTD-PML algorithm reduces to the usual nonlinear dispersive FDTD algorithm.

I. INTRODUCTION

With the advent of high power computers that provide fast execution times and great quantities of computer memory, we are at the stage where we can perform direct numerical calculations of Maxwell's equations in nonlinear dispersive materials. Out of many numerical techniques available in the computational electromagnetic community, one that has shown a great promise in the time domain is the well-known finite-difference time-domain (FDTD) method [1]. It is based on using a simple staggered differencing scheme in both time and space to calculate the transient behavior of electromagnetic field quantities. One of the greatest challenges of the FDTD methods has been the efficient and accurate formulation of electromagnetic wave interactions in unbounded regions. For such problems, an absorbing boundary condition must be introduced at the outer layer boundary to simulate the extension of the lattice to infinity. One approach that has given a great promise in realizing such an absorbing outer boundary inside the finite volume computational domain is the well-known perfectly-matched-layer (PML) algorithm that was first introduced by J. P. Berenger [2] in 1994 for the free space boundary. Since that time Chew and Weedon [3] came up with the modified PML algorithm that is based on complex coordinate stretching, which is shown to be equivalent to the anistropic PML medium approach [4].

In this paper, we explore the formulation of a 3-dimensional perfectly-matched-layer (PML) algorithm that is used to describe the behavior of electromagnetic quantities in outer absorbing boundary layers of a nonlinear dispersive medium which serves to absorb all outgoing waves within a finite computational volume. We consider the case where a plane wave propagates outwardly from a nonlinear dispersive medium to a nonlinear dispersive PML medium through a reflectionless PML interface. We start the analysis based on the extension of the unsplit-field uniaxial PML formulation [4-8] of Maxwell's equations that are obtained in the frequency domain inside the nonlinear dispersive PML medium. We perform the inverse Fourier transform of these equations from the frequency domain to the time domain in order to obtain a set of ordinary first-order differential equations. Then, these equations are finite differenced in both time and space using the usual staggered Yee FDTD scheme while expanding the electric and magnetic field vectors in time using the Taylor series expansion about the current time step to evaluate next time step values of the electromagnetic field quantities. Depending on the number of terms kept in the Taylor series expansion, we can numerically update the field values to any desired accuracy. In Section II, we use the piecewise-linear approximation, which is equivalent to using only the first-order, timedependent term of the Taylor series expansion, to show the process involved in obtaining a second-order accurate FDTD-PML algorithm. To obtain higher-order accurate FDTD-PML algorithms in time, we simply need to include higher-order, time-dependent terms in the Taylor series expansion and follow the same steps shown in Section II.

In the absence of the PML interface, the FDTD-PML algorithm reduces to the FDTD algorithm obtained for nonlinear dispersive media [9,10].

II. PML FORMULATION FOR NONLINEAR DISPERSIVE MEDIA

For a wave propagating into anisotropic, uniaxial nonlinear dispersive PML media, the modified Maxwell's equations under the PML formulation with stretched coordinates [3] can be expressed in the frequency domain (e^{iωt} convention) as

$$\underline{\nabla} \times \underline{E}(\omega; \underline{x}) = -i\omega \underline{S}^{PML}(\omega) \bullet \mu_0 \mu_R \underline{H}(\omega; \underline{x}), \qquad (2.1)$$

$$\underline{\nabla} \times \underline{\mathbf{H}}(\omega; \underline{\mathbf{x}}) = i\omega \underline{\mathbf{S}}^{\mathrm{PML}}(\omega) \bullet \underline{\mathbf{D}}(\omega; \underline{\mathbf{x}}), \qquad (2.2)$$

with

$$\underline{\underline{D}}(\omega;\underline{x}) = \varepsilon_0 \varepsilon_R \underline{\underline{E}}(\omega;\underline{x}) + \varepsilon_0 \sum_{\rho=1}^{\rho_{max}} \underline{\underline{P}}_{\rho}^{L}(\omega;\underline{x}) + \varepsilon_0 \sum_{\rho=1}^{\rho_{max}} \underline{\underline{P}}_{\rho}^{NL}(\omega;\underline{x}) , \qquad (2.3)$$

$$\underline{P}_{\rho}^{L}(\omega;\underline{x}) = \mathcal{F}\left\{\underline{P}_{\rho}^{L}(t;\underline{x})\right\} = \mathcal{F}\left\{\int_{-\infty}^{\infty} d\tau \ X_{\rho}^{L}(t-\tau) \ \underline{E}(\tau;\underline{x})\right\} = X_{\rho}^{L}(\omega) \ \underline{E}(\omega;\underline{x}), \tag{2.4}$$

$$\underline{P}_{\rho}^{NL}(\omega;\underline{x}) = \mathcal{F}\left\{\underline{E}(t;\underline{x}) R_{\rho}^{NL}(t;\underline{x})\right\} = \mathcal{F}\left\{\underline{E}(t;\underline{x}) \int_{-\infty}^{\infty} d\tau X_{\rho}^{NL}(t-\tau) [\underline{E}(\tau;\underline{x}) \bullet \underline{E}(\tau;\underline{x})]\right\}, \tag{2.5}$$

where $\underline{E}(\omega;x)$ is the electric field vector, $\underline{H}(\omega;\underline{x})$ is the magnetic field vector, $\underline{D}(\omega;\underline{x})$ is the displacement field vector, $\underline{P}_{\rho}^{L}(\omega;\underline{x})$ is the linear (first-order) electric polarization vector, $\underline{P}_{\rho}^{NL}(\omega;\underline{x})$ is the nonlinear (third-order) electric polarization vector, $\underline{S}^{PML}(\omega)$ is the uniaxial anisotropic PML matrix, ε_{o} is the free space electric permittivity, ε_{R} is the relative permittivity, μ_{0} is the free-space permeability, μ_{R} is the relative permeability, $\mu_{\rho}^{NL}(t)$ and $\mu_{\rho}^{NL}(t)$ are the $\mu_{\rho}^{NL}(t)$ are the $\mu_{\rho}^{NL}(t)$ is the maximum number of terms which we choose to consider for a particular formulation of Eq. (2.3). In Eq. (2.5) $\mu_{\rho}^{NL}(t;\underline{x})$ is introduced to isolate the part of $\mu_{\rho}^{NL}(t;\underline{x})$ that is represented by a convolution function. Also used in the above equations are notations • and $\mu_{\rho}^{NL}(t;\underline{x})$ denoting a dot product and the Fourier transform operation. Elements of the uniaxial anisotropic PML matrix, $\mu_{\rho}^{NL}(t;\underline{x})$ is given by

$$\underline{\underline{S}}^{PML}(\omega) = \begin{pmatrix} \frac{S_{y}(\omega) S_{z}(\omega)}{S_{x}(\omega)} & 0 & 0\\ 0 & \frac{S_{x}(\omega) S_{z}(\omega)}{S_{y}(\omega)} & 0\\ 0 & 0 & \frac{S_{x}(\omega) S_{y}(\omega)}{S_{z}(\omega)} \end{pmatrix}, \tag{2.6}$$

where $S_x(\omega)$, $S_y(\omega)$ and $S_z(\omega)$ are arbitrarily defined ω -dependent functions that satisfy the impedance matching condition at the interface of the non-PML medium and the PML medium. It is a common practice in the FDTD community to choose $S_x(\omega)$, $S_y(\omega)$ and $S_z(\omega)$ in the following forms:

$$S_x(\omega) = 1 + \frac{\sigma_x}{i\omega\varepsilon_0\varepsilon_R} \text{ with } \frac{\sigma_x}{\varepsilon_0\varepsilon_R} = \frac{\sigma_x^*}{\mu_0\mu_R},$$
 (2.7-2.8)

$$S_{y}(\omega) = 1 + \frac{\sigma_{y}}{i\omega\varepsilon_{0}\varepsilon_{R}} \text{ with } \frac{\sigma_{y}}{\varepsilon_{0}\varepsilon_{R}} = \frac{\sigma_{y}^{*}}{\mu_{0}\mu_{R}}, \text{ and}$$
 (2.9-2.10)

$$S_z(\omega) = 1 + \frac{\sigma_z}{i\omega\varepsilon_0\varepsilon_R} \text{ with } \frac{\sigma_z}{\varepsilon_0\varepsilon_R} = \frac{\sigma_z^*}{\mu_0\mu_R},$$
 (2.11-2.12)

where σ_x , σ_y and σ_z are the PML electric conductivities, and σ_x^* , σ_y^* and σ_z^* are the PML magnetic conductivities with subscripts x, y and z denoting the directions in which PML conductivities are assigned [2]. These PML conductivities are introduced arbitrarily in order to implement the FDTD-PML algorithm.

We first eliminate $\underline{D}(\underline{\omega};\underline{x})$ in favor of expressing Maxwell's equations in terms of $\underline{E}(\underline{\omega};\underline{x})$, $\underline{P}_{\rho}^{L}(\underline{\omega};\underline{x})$ and $\underline{P}_{\rho}^{NL}(\underline{\omega};\underline{x})$ by substituting Eq. (2.3) into Eq. (2.2). Upon taking the inverse Fourier transforms of Eqs. (2.1), (2.2), (2.4) and (2.5) and using the expressions shown in Eqs. (2.7) through (2.12), we obtain the following time-dependent equations:

$$\mu_0 \mu_R \frac{\partial \underline{\underline{H}}(t;\underline{x})}{\partial t} + \mu_0 \mu_R \underline{\underline{\Psi_0}} \bullet \underline{\underline{H}}(t;\underline{x}) + \mu_0 \mu_R \underline{\underline{\Psi_1}} \bullet \underline{\underline{H}}^{Delay}(t;\underline{x}) + \underline{\nabla} \underline{x} \underline{\underline{E}}(t;\underline{x}) = 0, \qquad (2.13)$$

$$\varepsilon_{0}\varepsilon_{R} \frac{\partial \underline{E}(t;\underline{x})}{\partial t} + \varepsilon_{0} \sum_{\rho} \frac{\partial \underline{P}_{\rho}^{L}(t;\underline{x})}{\partial t} + \varepsilon_{0} \sum_{\rho} \frac{\partial [\underline{E}(t;\underline{x}) R_{\rho}^{NL}(t;\underline{x})]}{\partial t} \\
+ \varepsilon_{0} \underline{\underline{\Psi}_{0}} \bullet \left[\varepsilon_{R}\underline{E}(t;\underline{x}) + \sum_{\rho} \underline{P}_{\rho}^{L}(t;\underline{x}) + \underline{E}(t;\underline{x}) \sum_{\rho} R_{\rho}^{NL}(t;\underline{x})\right] \\
+ \varepsilon_{0} \underline{\underline{\Psi}_{1}} \bullet \left[\varepsilon_{R}\underline{E}^{Delay}(t;\underline{x}) + \sum_{\rho} \underline{P}_{\rho}^{LDelay}(t;\underline{x}) + \sum_{\rho} \underline{P}_{\rho}^{NLDelay}(t;\underline{x})\right] - \underline{\nabla} \underline{x} \underline{H}(t;\underline{x}) = 0, \quad (2.14)$$

with

$$\underline{P}_{\rho}^{L}(t;\underline{x}) = \int_{-\infty}^{\infty} d\tau \ X_{\rho}^{L}(t-\tau) \, \underline{E}(\tau;\underline{x}) , \qquad (2.15)$$

$$R_{\rho}^{NL}(t;\underline{x}) = \int_{-\infty}^{\infty} d\tau \, X_{\rho}^{NL}(t-\tau) \left[\underline{E}(\tau;\underline{x}) \bullet \underline{E}(\tau;\underline{x}) \right], \tag{2.16}$$

$$\underline{\underline{H}}^{Delay}(t;\underline{x}) = \int_{-\infty}^{t} d\tau \, \underline{\underline{\Phi}}(t-\tau) \bullet \underline{\underline{H}}(\tau;\underline{x}), \qquad (2.17)$$

$$\underline{\underline{E}}^{\text{Delay}}(t;\underline{x}) = \int_{-\infty}^{t} d\tau \, \underline{\underline{\Phi}}(t-\tau) \bullet \underline{\underline{E}}(\tau;\underline{x}), \qquad (2.18)$$

$$\underline{\underline{P}}_{\rho}^{\text{LDelay}}(t;\underline{\underline{x}}) = \int_{-\infty}^{t} d\tau \, \underline{\underline{\Phi}}(t-\tau) \bullet \underline{\underline{P}}_{\rho}^{L}(\tau;\underline{\underline{x}}), \qquad (2.19)$$

$$\underline{\underline{P}}_{\rho}^{\text{NLDelay}}(t;\underline{x}) = \int_{-\infty}^{t} d\tau \, \underline{\underline{\Phi}}(t-\tau) \bullet [\underline{\underline{E}}(\tau,x) \, R_{\rho}^{\text{NL}}(\tau;\underline{x})], \qquad (2.20)$$

where

$$\underline{\underline{\Psi}_{0}} = \begin{pmatrix} \left(\frac{\sigma_{y}}{\epsilon_{0}\varepsilon_{R}} + \frac{\sigma_{z}}{\epsilon_{0}\varepsilon_{R}} - \frac{\sigma_{x}}{\epsilon_{0}\varepsilon_{R}}\right) & 0 & 0 \\ 0 & \left(\frac{\sigma_{x}}{\epsilon_{0}\varepsilon_{R}} + \frac{\sigma_{z}}{\epsilon_{0}\varepsilon_{R}} - \frac{\sigma_{y}}{\epsilon_{0}\varepsilon_{R}}\right) & 0 \\ 0 & 0 & \left(\frac{\sigma_{x}}{\epsilon_{0}\varepsilon_{R}} + \frac{\sigma_{y}}{\epsilon_{0}\varepsilon_{R}} - \frac{\sigma_{z}}{\epsilon_{0}\varepsilon_{R}}\right) \end{pmatrix}, (2.21)$$

$$\underline{\Psi}_{1} = \begin{pmatrix}
\left(\frac{\sigma_{y}}{\epsilon_{0}\epsilon_{R}} - \frac{\sigma_{x}}{\epsilon_{0}\epsilon_{R}}\right) & \sigma_{z} - \frac{\sigma_{x}}{\epsilon_{0}\epsilon_{R}} & 0 \\
0 & \left(\frac{\sigma_{x}}{\epsilon_{0}\epsilon_{R}} - \frac{\sigma_{y}}{\epsilon_{0}\epsilon_{R}}\right) & \sigma_{z} - \frac{\sigma_{y}}{\epsilon_{0}\epsilon_{R}} & 0 \\
0 & 0 & \left(\frac{\sigma_{x}}{\epsilon_{0}\epsilon_{R}} - \frac{\sigma_{z}}{\epsilon_{0}\epsilon_{R}}\right) & \sigma_{z} - \frac{\sigma_{z}}{\epsilon_{0}\epsilon_{R}} & \sigma_{z} \\
0 & 0 & \left(\frac{\sigma_{x}}{\epsilon_{0}\epsilon_{R}} - \frac{\sigma_{z}}{\epsilon_{0}\epsilon_{R}}\right) & \sigma_{z} - \frac{\sigma_{z}}{\epsilon_{0}\epsilon_{R}} & \sigma_{z} \\
0 & 0 & \left(\frac{\sigma_{x}}{\epsilon_{0}\epsilon_{R}} - \frac{\sigma_{z}}{\epsilon_{0}\epsilon_{R}}\right) & \sigma_{z} - \frac{\sigma_{z}}{\epsilon_{0}\epsilon_{R}} & \sigma_{z} \\
0 & 0 & \left(\frac{\sigma_{x}}{\epsilon_{0}\epsilon_{R}} - \frac{\sigma_{z}}{\epsilon_{0}\epsilon_{R}}\right) & \sigma_{z} - \frac{\sigma_{z}}{\epsilon_{0}\epsilon_{R}} & \sigma_{z} - \frac{\sigma_{z}}{\epsilon_$$

$$\underline{\underline{\Phi}}(t-\tau) = \begin{pmatrix} \exp[-(\frac{\sigma_x}{\varepsilon_0 \varepsilon_R})(t-\tau)] & 0 & 0 \\ 0 & \exp[-(\frac{\sigma_y}{\varepsilon_0 \varepsilon_R})(t-\tau)] & 0 \\ 0 & 0 & \exp[-(\frac{\sigma_z}{\varepsilon_0 \varepsilon_R})(t-\tau)] \end{pmatrix}. \tag{2.23}$$

In the above, $\underline{H}^{Delay}(t;\underline{x})$, $\underline{E}^{Delay}(t;\underline{x})$, $\underline{P}_{\rho}^{LDelay}(t;\underline{x})$ and $\underline{P}_{\rho}^{NLDelay}(t;\underline{x})$ are introduced to handle the delayed time-response behavior of $\underline{H}(t;\underline{x})$, $\underline{E}(t;\underline{x})$, $\underline{P}_{\rho}^{L}(t;x)$ and $[\underline{E}(t;\underline{x})R_{\rho}^{NL}(t;\underline{x})]$, respectively. These functions follow naturally from taking the inverse Fourier transforms of convolution functions $[1/(i\omega \underline{I} + \underline{A})]\underline{H}(\omega;\underline{x})$, $[1/(i\omega \underline{I} + \underline{A})]\underline{P}_{\rho}^{L}(\omega;\underline{x})$ and $[1/(i\omega \underline{I} + \underline{A})]\underline{P}_{\rho}^{NL}(\omega;\underline{x})$ by realizing the inverse Fourier transform of $[1/(i\omega \underline{I} + \underline{A})]$ is given by $\exp(-\underline{A}t)$, where \underline{I} is the identity matrix and \underline{A} is a time independent diagonal matrix expressed as diag $[\sigma_x/(\varepsilon_0\varepsilon_R), \sigma_y/(\varepsilon_0\varepsilon_R), \sigma_z/(\varepsilon_0\varepsilon_R)]$.

To solve Eqs. (2.13) through (2.20), we need to specify expressions for linear and nonlinear electric susceptibility functions. In this paper we consider the case in which both the linear and nonlinear electric susceptibility functions are expressed as complex functions that contain complex constant coefficients and exhibit exponential behavior in the time domain as follows:

$$X_{\rho}^{L}(t) = \operatorname{Re}\left\{\alpha_{\rho}^{L} \exp\left[-(\gamma_{\rho}^{L})t\right]\right\} U(t), \qquad (2.24)$$

and

$$X_{\rho}^{NL}(t) = \text{Re}\left\{\alpha_{\rho}^{NL} \exp[-(\gamma_{\rho}^{NL})t]\right\} U(t),$$
 (2.25)

where Re{ } is used to represent the real part of a complex function, U(t) is the unit step function, and α_p^L , γ_0^L , α_p^{NL} and γ_0^{NL} are complex constant coefficients. Now Eqs. (2.15) and (2.16) are expressed in the following forms:

$$\underline{\underline{P}}_{\rho}^{L}(t;\underline{x}) = \operatorname{Re}\left\{\underline{\underline{Q}}_{\rho}^{L}(t;\underline{x})\right\} = \operatorname{Re}\left\{\alpha_{\rho}^{L}\int_{-\infty}^{t} d\tau \exp[-(\gamma_{\rho}^{L})(t-\tau)]\underline{\underline{E}}(\tau;\underline{x})\right\},\tag{2.26}$$

and

$$R_{\rho}^{NL}(t;\underline{x}) \equiv \operatorname{Re}\left\{Q_{\rho}^{NL}(t;\underline{x})\right\} = \operatorname{Re}\left\{\alpha_{\rho}^{NL}\int_{-\infty}^{t}d\tau \exp[-(\gamma_{\rho}^{NL})(t-\tau)]\left[\underline{E}(\tau;\underline{x})\bullet\underline{E}(\tau;\underline{x})\right]\right\},\tag{2.27}$$

where complex functions $Q_{\rho}^{L}(t;\underline{x})$ and $Q_{\rho}^{NL}(t;\underline{x})$ are introduced in the above equations such that the real parts of these complex functions result in $\underline{P}_{\rho}^{L}(t;\underline{x})$ and $R_{\rho}^{NL}(t;\underline{x})$, respectively.

We need to point out that by making the proper choices of complex constant coefficients and performing

the Fourier transforms of Eqs. (2.24) and (2.25), we can readily obtain the familiar constant conductivity [i.e., α_{ρ}^{L} is real, $\gamma_{\rho}^{L} = 0$, $\alpha_{\rho}^{NL} = 0$ and $\gamma_{\rho}^{NL} = 0$], Debye [i.e., α_{ρ}^{L} , γ_{ρ}^{L} , α_{ρ}^{NL} and γ_{ρ}^{NL} are all real] and Lorentz [i.e., α_0^L and α_0^{NL} are both imaginary, and γ_0^L are both real] forms of the complex permittivity in the frequency domain.

To derive FDTD expressions based on Yee FDTD scheme, Eqs. (2.13), (2.14), (2.25), (2.26) and (2.17) through (2.20) have to be solved numerically for $\underline{H}(t;\underline{x})$, $\underline{E}(t;\underline{x})$, $Q_{\rho}^{L}(t;\underline{x})$, $Q_{\rho}^{NL}(t;\underline{x})$, $\underline{H}^{Delay}(t;\underline{x})$, $\underline{E}^{Delay}(t;\underline{x})$, $\underline{P}_{\rho}^{LDelay}(t;\underline{x})$ and $\underline{P}_{\rho}^{NLDelay}(t;\underline{x})$ at each time step by correctly carrying out the numerical integration of convolution integrals $Q_{\rho}^{L}(t;\underline{x})$, $Q_{\rho}^{NL}(t;\underline{x})$, $\underline{H}^{Delay}(t;\underline{x})$, $\underline{E}^{Delay}(t;\underline{x})$, $\underline{P}_{\rho}^{LDelay}(t;\underline{x})$ and $\underline{P}_{\rho}^{NLDelay}(t;\underline{x})$. Therefore, the whole solution rests on the question of how to carry out the numerical integration of $Q_{\rho}^{L}(t;\underline{x})$, $Q_{\rho}^{NL}(t;\underline{x})$

$$\frac{\partial \underline{Q}_{\rho}^{L}(t;\underline{x})}{\partial t} + (\gamma_{\rho}^{L})\underline{Q}_{\rho}^{L}(t;\underline{x}) = \alpha_{\rho}^{L}\underline{E}(t;\underline{x}), \qquad (2.28)$$

$$\frac{\partial Q_{\rho}^{NL}(t;\underline{x})}{\partial t} + (\gamma_{\rho}^{NL}) Q_{\rho}^{NL}(t;\underline{x}) = \alpha_{\rho}^{NL} [\underline{E}(t;\underline{x}) \bullet \underline{E}(t;\underline{x})], \qquad (2.29)$$

$$\frac{\partial \underline{\underline{H}}^{Delay}(t;\underline{\underline{x}})}{\partial t} + \underline{\underline{\Phi}}(t) \bullet \underline{\underline{H}}^{Delay}(t;\underline{\underline{x}}) = \underline{\underline{H}}(t;\underline{\underline{x}}), \qquad (2.30)$$

$$\frac{\partial \underline{E}^{\text{Delay}}(t;\underline{x})}{\partial t} + \underline{\Phi}(t) \bullet \underline{E}^{\text{Delay}}(t;\underline{x}) = \underline{E}(t;\underline{x}), \qquad (2.31)$$

$$\frac{\partial \underline{Q}_{\rho}^{\text{LDelay}}(t;\underline{x})}{\partial t} + \underline{\Phi}(t) \bullet \underline{Q}_{\rho}^{\text{LDelay}}(t;\underline{x}) = \underline{Q}_{\rho}^{L}(t;\underline{x}), \qquad (2.32)$$

$$\frac{\partial \underline{Q}_{\rho}^{\text{NLDelay}}(t;\underline{x})}{\partial t} + \underline{\Phi}(t) \bullet \underline{Q}_{\rho}^{\text{NLDelay}}(t;\underline{x}) = \underline{E}(t;\underline{x}) \, Q_{\rho}^{\text{NL}}(t;\underline{x}), \qquad (2.33)$$

where complex functions $Q_{\rho}^{\text{LDelay}}(t;\underline{x})$ and $Q_{\rho}^{\text{NLDelay}}(t;\underline{x})$ are introduced in Eqs. (2.32) and (2.33) such that the real parts of these complex functions result in $\underline{P}_{\rho}^{\text{LDelay}}(t;\underline{x})$ and $\underline{P}_{\rho}^{\text{NLDelay}}(t;\underline{x})$, respectively.

To show how we can use Eqs. (2.13), (2.14) and (2.28) through (2.33) to come up with a 3-D FDTD-PML algorithm for nonlinear dispersive PML media, we integrate Eqs. (2.13) and (2.30) from $t=(n-\frac{1}{2})\Delta t$, and Eqs. (2.14), (2.28), (2.29) and (2.31) through (2.33) from $t=n\Delta t$ to $t=(n+1)\Delta t$. Then Eqs. (2.28) through (2.33) are solved exactly using the integrating factor technique for a given discrete time interval to go forward in time by Δt . The result is that we need to perform definite integrals that appear in the following equations:

$$\mu_{0}\mu_{R} \int_{(n-\frac{1}{2})\Delta t}^{(n+\frac{1}{2})\Delta t} d\tau \frac{\partial \underline{\underline{H}}(\tau;\underline{x})}{\partial \tau} + \mu_{0}\mu_{R} \underline{\underline{\Psi}_{0}} \bullet \int_{(n-\frac{1}{2})\Delta t}^{(n+\frac{1}{2})\Delta t} d\tau \underline{\underline{H}}(\tau;\underline{x})$$

$$+ \mu_{0}\mu_{R} \underline{\underline{\Psi}_{1}} \bullet \int_{(n-\frac{1}{2})\Delta t}^{(n+\frac{1}{2})\Delta t} d\tau \underline{\underline{H}}^{Delay}(\tau;\underline{x}) + \int_{(n-\frac{1}{2})\Delta t}^{(n+\frac{1}{2})\Delta t} d\tau \underline{\underline{\nabla}} \underline{x} \underline{\underline{E}}(\tau;\underline{x}) = 0, \qquad (2.34)$$

$$\begin{split} & \epsilon_{0}\epsilon_{R} \int_{n\Delta t}^{(n+1)\Delta t} d\tau \, \frac{\partial \underline{E}(\tau;\underline{x})}{\partial \, \tau} + \epsilon_{0} \, Re \big\{ \sum_{\rho} \int_{n\Delta t}^{(n+1)\Delta t} d\tau \, \frac{\partial \underline{Q}_{\rho}^{L}(\tau;\underline{x})}{\partial \, \tau} \big\} + \epsilon_{0} \, Re \big\{ \sum_{\rho} \int_{n\Delta t}^{(n+1)\Delta t} d\tau \, \frac{\partial [\underline{E}(\tau;\underline{x}) \, Q_{\rho}^{NL}(\tau;\underline{x})]}{\partial \, \tau} \big\} \\ & + \epsilon_{0}\epsilon_{R} \underline{\Psi_{0}} \bullet \int_{n\Delta t}^{(n+1)\Delta t} \underline{E}(\tau;\underline{x}) \, + \epsilon_{0} \underline{\Psi_{0}} \bullet Re \, \big\{ \sum_{\rho} \int_{n\Delta t}^{(n+1)\Delta t} d\tau \, \underline{Q}_{\rho}^{L}(\tau;\underline{x}) \big\} \\ & + \epsilon_{0}\underline{\Psi_{0}} \bullet Re \big\{ \sum_{\rho} \int_{n\Delta t}^{(n+1)\Delta t} \underline{E}(\tau;\underline{x}) \, Q_{\rho}^{NL}(\tau;\underline{x}) \big\} + \epsilon_{0}\epsilon_{R} \underline{\Psi_{1}} \bullet Re \big\{ \sum_{\rho} \int_{n\Delta t}^{(n+1)\Delta t} \underline{d\tau} \, \underline{E}^{Delay}(\tau;\underline{x}) \\ & + \epsilon_{0}\underline{\Psi_{1}} \bullet Re \big\{ \sum_{\rho} \int_{n\Delta t}^{(n+1)\Delta t} \underline{d\tau} \, \underline{Q}_{\rho}^{LDelay}(\tau;\underline{x}) \big\} + \epsilon_{0}\underline{\Psi_{1}} \bullet Re \big\{ \sum_{\rho} \int_{n\Delta t}^{(n+1)\Delta t} \underline{d\tau} \, \underline{Q}_{\rho}^{NLDelay}(\tau;\underline{x}) \big\} \\ & - \int_{0}^{(n+1)\Delta t} \underline{d\tau} \, \underline{V} \, \underline{X} \, \underline{H}(\tau;\underline{x}) = 0 \,, \end{split} \tag{2.35}$$

$$\underline{Q}_{\rho}^{L}(n\Delta t + \Delta t; \underline{x}) = \exp[-(\gamma_{\rho}^{L})\Delta t] \left[\underline{Q}_{\rho}^{L}(n\Delta t; \underline{x}) + \alpha_{\rho}^{L} \int_{n\Delta t}^{(n+1)\Delta t} d\tau \exp[-(\gamma_{\rho}^{L})(n\Delta t - \tau)] \underline{E}(\tau; \underline{x}) \right], \tag{2.36}$$

$$Q_{\rho}^{NL}(n\Delta t + \Delta t; \underline{x}) = \exp[-(\gamma_{\rho}^{NL})\Delta t] \left[Q_{\rho}^{NL}(n\Delta t; \underline{x}) + \alpha_{\rho}^{NL} \int_{0}^{(n+1)\Delta t} d\tau \exp[-(\gamma_{\rho}^{NL})(n\Delta t - \tau)] \left[\underline{E}(\tau; \underline{x}) \bullet \underline{E}(\tau; \underline{x}) \right] \right],$$
(2.37)

$$\underline{\underline{H}}^{\text{Delay}}(n\Delta t + \frac{1}{2}\Delta t; \underline{x}) = \exp(-\underline{\Phi}\Delta t) \bullet \left[\underline{\underline{H}}^{\text{Delay}}(n\Delta t - \frac{1}{2}\Delta t; \underline{x}) + \int_{(n-\frac{1}{2}\Delta t)\Delta t}^{(n+\frac{1}{2}\Delta t)} d\tau \exp[-\underline{\Phi}(n\Delta t - \frac{1}{2}\Delta t - \tau)] \bullet \underline{\underline{H}}(\tau; \underline{x})\right], \tag{2.38}$$

$$\underline{\underline{E}}^{\text{Delay}}(n\Delta t + \Delta t; \underline{\underline{x}}) = \exp(-\underline{\underline{\Phi}}\Delta t) \bullet \left[\underline{\underline{E}}^{\text{Delay}}(n\Delta t; \underline{\underline{x}}) + \int_{n\Delta t}^{(n+1)\Delta t} d\tau \exp[-\underline{\underline{\Phi}}(n\Delta t - \tau)] \bullet \underline{\underline{E}}(\tau; \underline{\underline{x}})\right], \tag{2.39}$$

$$\begin{split} & \underline{Q}_{\rho}^{LDelay}(n\Delta t + \Delta t; \underline{x}) = exp(-\underline{\Phi}\Delta t) \bullet \left[\underline{Q}_{\rho}^{LDelay}(n\Delta t; \underline{x}) + \int_{n\Delta t}^{(n+1)\Delta t} d\tau \exp[-\underline{\Phi}(n\Delta t - \tau)] \bullet \underline{Q}_{\rho}^{L}(\tau; \underline{x}) \right] \\ & = exp(-\underline{\Phi}\Delta t) \bullet \left[\underline{Q}_{\rho}^{LDelay}(n\Delta t; \underline{x}) + \int_{n\Delta t}^{(n+1)\Delta t} d\tau \exp[-\underline{\Phi}(n\Delta t - \tau) - \underline{I}_{\underline{x}}(\gamma_{\rho}^{L})(\tau - n\Delta t)] \bullet \underline{Q}_{\rho}^{L}(n\Delta t; \underline{x}) \right] \\ & + \alpha_{\rho}^{L} \int_{n\Delta t}^{(n+1)\Delta t} d\tau \int_{n\Delta t}^{\tau} d\tau' \exp[-\underline{\Phi}(n\Delta t - \tau) - \underline{I}_{\underline{x}}(\gamma_{\rho}^{L})(\tau - \tau')] \bullet \underline{E}(\tau'; \underline{x}) \right], \end{split} \tag{2.40}$$

Furthermore, some of the definite integrals that appear in Eqs. (2.34) and (2.35) are manipulated and cast in the following forms:

$$\int_{(n-\frac{1}{2})\Delta t}^{(n+\frac{1}{2})\Delta t} d\tau \, \underline{\underline{H}}^{Delay}(\tau;\underline{\underline{x}}) = \int_{(n-\frac{1}{2})\Delta t}^{(n+\frac{1}{2})\Delta t} d\tau \exp[-\underline{\underline{\Phi}}(\tau - n\Delta t + \frac{1}{2}\Delta t)] \bullet \underline{\underline{H}}^{Delay}(n\Delta t - \frac{1}{2}\Delta t;\underline{\underline{x}})$$

$$+ \int_{(n-\frac{1}{2})\Delta t}^{(n+\frac{1}{2})\Delta t} \int_{(n-\frac{1}{2})\Delta t}^{\tau} d\tau' \exp[-\underline{\underline{\Phi}}(\tau - \tau')] \bullet \underline{\underline{H}}(\tau';\underline{\underline{x}}), \qquad (2.42)$$

$$\int_{n\Delta t}^{(n+1)\Delta t} d\tau \, \underline{Q}_{\rho}^{L}(\tau; \underline{x}) = \int_{n\Delta t}^{(n+1)\Delta t} d\tau \exp[-(\gamma_{\rho}^{L})(\tau - n\Delta t)] \, \underline{Q}_{\rho}^{L}(n\Delta t; \underline{x})$$

$$+ \alpha_{\rho}^{L} \int_{n\Delta t}^{(n+1)\Delta t} d\tau \int_{n\Delta t}^{\tau} d\tau' \exp[-(\gamma_{\rho}^{L})(\tau - \tau')] \, \underline{E}(\tau'; \underline{x}), \qquad (2.43)$$

$$\int_{n\Delta t}^{(n+1)\Delta t} d\tau \, \underline{\underline{E}}(\tau;\underline{x}) \, Q_{\rho}^{NL}(\tau;\underline{x}) = \int_{n\Delta t}^{(n+1)\Delta t} d\tau \, \underline{\underline{E}}(\tau;\underline{x}) \, \exp[-(\gamma_{\rho}^{NL})(\tau-n\Delta t)] \, Q_{\rho}^{NL}(n\Delta t;\underline{x}) \\ + \alpha_{\rho}^{NL} \int_{n\Delta t}^{(n+1)\Delta t} \int_{n\Delta t}^{\tau} d\tau' \exp[-(\gamma_{\rho}^{NL})(\tau-\tau')] \, \underline{\underline{E}}(\tau;\underline{x}) \, [\underline{\underline{E}}(\tau';\underline{x}) \bullet \underline{\underline{E}}(\tau';\underline{x})] \,, \tag{2.44}$$

$$\int_{n\Delta t}^{(n+1)\Delta t} d\tau \, \underline{E}^{Delay}(\tau; \underline{x}) = \int_{n\Delta t}^{(n+1)\Delta t} d\tau \exp\left[-\underline{\underline{\Phi}}(\tau - n\Delta t)\right] \bullet \underline{E}^{Delay}(n\Delta t; \underline{x}) + \int_{n\Delta t}^{(n+1)\Delta t} d\tau \int_{n\Delta t}^{\tau} d\tau' \exp\left[-\underline{\underline{\Phi}}(\tau - \tau')\right] \bullet \underline{E}(\tau'; \underline{x}),$$
(2.45)

$$\int_{n\Delta t}^{(n+1)\Delta t} d\tau \underbrace{Q_{\rho}^{LDelay}(\tau;\underline{x})}_{n\Delta t} = \int_{n\Delta t}^{(n+1)\Delta t} d\tau \exp[-\underline{\underline{\Phi}}(\tau - n\Delta t)] \bullet \underbrace{Q_{\rho}^{LDelay}}_{\rho}(n\Delta t;\underline{x})$$

$$+ \int_{n\Delta t}^{(n+1)\Delta t} d\tau \int_{n\Delta t}^{\tau} d\tau' \exp[-\underline{\underline{\Phi}}\tau - \underline{\underline{I}}(\gamma_{\rho}^{L})(\tau' - n\Delta t)] \bullet \underbrace{Q_{\rho}^{L}}_{\rho}(n\Delta t;\underline{x})$$

$$+ \alpha_{\rho}^{L} \int_{n\Delta t}^{(n+1)\Delta t} d\tau \int_{n\Delta t}^{\tau} d\tau' \exp[-\underline{\underline{\Phi}}\tau - \underline{\underline{I}}(\gamma_{\rho}^{L})(\tau' - \tau'')] \bullet \underline{\underline{E}}(\tau'';\underline{x}), \qquad (2.46)$$

$$\int_{n\Delta t}^{(n+1)\Delta t} d\tau \, \underline{Q}_{\rho}^{NLDelay}(\tau; \underline{x}) = \int_{n\Delta t}^{(n+1)\Delta t} d\tau \, \exp[-\underline{\underline{\Phi}} \, (\tau - n\Delta t)] \bullet \, \underline{\underline{Q}}_{\rho}^{NLDelay}(n\Delta t; \underline{x})$$

$$+ \int_{n\Delta t}^{(n+1)\Delta t} \int_{n\Delta t}^{\tau} d\tau' \exp[-\underline{\underline{\Phi}} \, \tau - \underline{\underline{I}} \, (\gamma_{\rho}^{NL})(\tau' - n\Delta t)] \bullet \, \underline{\underline{E}}(\tau'; \underline{x}) \, \underline{Q}_{\rho}^{NL}(n\Delta t; \underline{x})$$

$$+ \alpha_{\rho}^{NL} \int_{n\Delta t}^{(n+1)\Delta t} \int_{n\Delta t}^{\tau} d\tau' \int_{n\Delta t}^{\tau} d\tau'' \exp[-\underline{\underline{\Phi}} \, \tau - \underline{\underline{I}} \, (\gamma_{\rho}^{NL})(\tau' - \tau'')] \bullet \, \underline{\underline{E}}(\tau'; \underline{x}) \, [\underline{\underline{E}}(\tau''; \underline{x}) \bullet \, \underline{\underline{E}}(\tau''; \underline{x})] \, . \tag{2.47}$$

To obtain second-order accuracy in time from a finite differencing technique, $\underline{\underline{H}}(t;\underline{x})$ and $\underline{\underline{E}}(t;\underline{x})$ are taken to be piecewise-linear continuous functions over the entire temporal integration range such that $\underline{\underline{H}}(t;\underline{x})$ and $\underline{\underline{E}}(t;\underline{x})$ change linearly with respect to time over given discrete time step intervals. It is equivalent to saying that we use only the first-order, time-dependent term of the Taylor series expansion for $\underline{\underline{H}}(t;\underline{x})$ and $\underline{\underline{E}}(t;\underline{x})$, respectively, that are expanded in time about the current time step of $t=(n-\frac{1}{2})\Delta t$ for $\underline{\underline{H}}(t;\underline{x})$ and the current time step of $t=n\Delta t$ for $\underline{\underline{E}}(t;\underline{x})$. Mathematically, we can express $\underline{\underline{H}}(t;\underline{x})$ and $\underline{\underline{E}}(t;\underline{x})$ in the following forms in terms of $(\underline{\underline{H}})_{ijk}^{n-\frac{1}{2}}$, $(\underline{\underline{H}})_{ijk}^{n-\frac{1}{2}}$, $(\underline{\underline{E}})_{ijk}^{n}$ and $(\underline{\underline{E}})_{ijk}^{n+1}$ where superscripts $n-\frac{1}{2}$, n, $n+\frac{1}{2}$ and n+1 are used to denote discrete time steps at $t=(n-\frac{1}{2})\Delta t$, $t=n\Delta t$, $t=(n+\frac{1}{2})\Delta t$ and $t=(n+1)\Delta t$, respectively. Subscripts are used to denote discrete spatial locations, $\underline{x}=[i\Delta x, j\Delta y, k\Delta z]$ for $\underline{\underline{E}}(t;\underline{x})$ and $\underline{x}=[(i-\frac{1}{2})\Delta x, (j-\frac{1}{2})\Delta y, (k-\frac{1}{2})\Delta z]$ for $\underline{\underline{H}}(t;\underline{x})$ with Δx , Δy and Δz being the spatial grid sizes in the x, y and z directions, respectively.

$$\underline{\underline{H}}(t;\underline{x}) = \begin{cases} (\underline{\underline{H}})_{ijk}^{n \to 1/2} + \frac{[(\underline{\underline{H}})_{ijk}^{n \to 1/2} - (\underline{\underline{H}})_{ijk}^{n \to 1/2}]}{\Delta t} [t - (n - 1/2)\Delta t] + \text{higher order terms,} \\ & \text{for } 0 \le (n - 1/2)\Delta t \le t \le (n + 1/2)\Delta t \end{cases}$$

$$(2.48)$$

$$0, \qquad \qquad \text{for } t < 0$$

$$\underline{\underline{E}}(t;\underline{x}) = \begin{cases} (\underline{\underline{E}})_{ijk}^{n} + \frac{[(\underline{\underline{E}})_{ijk}^{n+1} - (\underline{\underline{E}})_{ijk}^{n}]}{\Delta t} (t - n\Delta t) + \text{higher order terms,} \\ & \text{for } 0 \le n\Delta t \le t \le (n+1)\Delta t \end{cases}$$

$$(2.49)$$

$$0, \qquad \text{for } t < 0$$

Although we are not going to investigate higher than second-order accuracy in time in this paper, it is possible to obtain higher-order accurate FDTD algorithms by simply including more terms beyond the first-order, time-dependent term in the above Taylor series expansion.

Substituting Eqs. (2.48) and (2.49) into Eqs. (2.34) through (2.47) and performing the time integration from $t=(n-\frac{1}{2})\Delta t$ to $t=(n+\frac{1}{2})\Delta t$ for field values that depend on the magnetic field [i.e., $\underline{\underline{H}}(t;\underline{x})$ and $\underline{\underline{H}}^{Delay}(t;\underline{x})$], and from $t=n\Delta t$ to $t=(n+1)\Delta t$ for field values that depend on the electric field [i.e., $\underline{\underline{E}}(t;\underline{x})$, $Q_{\rho}^{LL}(t;\underline{x})$, $Q_{\rho}^{NLDelay}(t;\underline{x})$, $Q_{\rho}^{NLDelay}(t;\underline{x})$ and $Q_{\rho}^{NLDelay}(t;\underline{x})$, Eqs. (2.34) through (2.47) are cast into the following cubic algebraic expressions. These expressions are used to update field values $(\underline{\underline{H}})_{ijk}^{n+1}$, $(\underline{\underline{L}})_{ijk}^{n+1}$, $(\underline{\underline{L}})_$

$$\underline{\Omega_0} \bullet (\underline{H})_{ijk}^{n+1/2} + \underline{\Omega_1} \bullet (\underline{H})_{ijk}^{n-1/2} + \underline{\Omega_2} \bullet (\underline{H}^{Delay})_{ijk}^{n-1/2} + \underline{S_E} = 0, \qquad (2.50)$$

$$\begin{split} &\underbrace{(\underline{\Lambda}_{0})_{ijk}^{n}} \bullet (E)_{ijk}^{n+1} + (\underline{\Lambda}_{1})_{ijk}^{n} \bullet (E)_{ijk}^{n} + \text{Re} \left\{ \sum_{\rho} \frac{\Gamma_{\rho,0}^{L}}{\underline{\rho}_{\rho}} \bullet (\underline{Q}_{\rho}^{L})_{ijk}^{n} \right\} + \underline{\Omega}_{2} \bullet (\underline{E}^{\text{Delay}})_{ijk}^{n} \\ &+ \underline{\Omega}_{3} \bullet \text{Re} \left\{ \sum_{\rho} (\underline{Q}_{\rho}^{\text{LDelay}})_{ijk}^{n} \right\} + \underline{\Omega}_{3} \bullet \text{Re} \left\{ \sum_{\rho} (\underline{Q}_{\rho}^{\text{NLDelay}})_{ijk}^{n} \right\} \\ &+ \text{Re} \left\{ \sum_{\rho} \underline{\Gamma_{\rho,0}^{\text{NL}}} \right\} \bullet (\underline{E})_{ijk}^{n} \left[(\underline{E})_{ijk}^{n} \bullet (\underline{E})_{ijk}^{n} \right] + \text{Re} \left\{ \sum_{\rho} \underline{\Gamma_{\rho,1}^{\text{NL}}} \right\} \bullet (\underline{E})_{ijk}^{n} \left[(\underline{E})_{ijk}^{n} \bullet (\underline{E})_{ijk}^{n+1} \right] \\ &+ \text{Re} \left\{ \sum_{\rho} \underline{\Gamma_{\rho,2}^{\text{NL}}} \right\} \bullet (\underline{E})_{ijk}^{n} \left[(\underline{E})_{ijk}^{n+1} \bullet (\underline{E})_{ijk}^{n+1} \right] + \text{Re} \left\{ \sum_{\rho} \underline{\Gamma_{\rho,3}^{\text{NL}}} \right\} \bullet (\underline{E})_{ijk}^{n+1} \left[(\underline{E})_{ijk}^{n} \bullet (\underline{E})_{ijk}^{n+1} \right] \\ &+ \text{Re} \left\{ \sum_{\rho} \underline{\Gamma_{\rho,4}^{\text{NL}}} \right\} \bullet (\underline{E})_{ijk}^{n+1} \left[(\underline{E})_{ijk}^{n} \bullet (\underline{E})_{ijk}^{n+1} \right] + \text{Re} \left\{ \sum_{\rho} \underline{\Gamma_{\rho,5}^{\text{NL}}} \right\} \bullet (\underline{E})_{ijk}^{n+1} \left[(\underline{E})_{ijk}^{n+1} \bullet (\underline{E})_{ijk}^{n+1} \right] \\ &+ S_{H} = 0, \end{split} \tag{2.51}$$

$$(\underline{Q}_{0}^{L})_{ijk}^{n+1} = \Theta_{\rho,0}^{L} \left[(\underline{Q}_{0}^{L})_{ijk}^{n} + \Theta_{\rho,1}^{L} (\underline{E})_{ijk}^{n} + \Theta_{\rho,2}^{L} (\underline{E})_{ijk}^{n+1} \right], \tag{2.52}$$

$$(Q_{\rho}^{NL})_{ijk}^{n+1} = \Theta_{\rho,0}^{NL} \left[(Q_{\rho}^{NL})_{ijk}^{n} + \Theta_{\rho,1}^{NL} \left[(\underline{E})_{ijk}^{n} \bullet (\underline{E})_{ijk}^{n} \right] + \Theta_{\rho,2}^{NL} \left[(\underline{E})_{ijk}^{n} \bullet (\underline{E})_{ijk}^{n+1} \right] + \Theta_{\rho,3}^{NL} \left[(\underline{E})_{ijk}^{n+1} \bullet (\underline{E})_{ijk}^{n+1} \right] \right],$$
(2.53)

$$(\underline{\mathbf{H}}^{\text{Delay}})_{ijk}^{n+1/2} = \underline{\Omega_4} \bullet \left[(\underline{\mathbf{H}}^{\text{Delay}})_{ijk}^{n-1/2} + \underline{\Omega_5} \bullet (\underline{\mathbf{H}})_{ijk}^{n-1/2} + \underline{\Omega_6} \bullet (\underline{\mathbf{H}})_{ijk}^{n+1/2} \right], \tag{2.54}$$

$$(\underline{E}^{\text{Delay}})_{ijk}^{n+1} = \underline{\Omega_4} \bullet \left[(\underline{E}^{\text{Delay}})_{ijk}^n + \underline{\Omega_5} \bullet (\underline{E})_{ijk}^n + \underline{\Omega_6} \bullet (\underline{E})_{ijk}^{n+1} \right], \tag{2.55}$$

$$(\underline{Q}_{\rho}^{\text{LDelay}})_{ijk}^{n+1} = \underline{\Omega_{4}} \bullet \left[(\underline{Q}_{\rho}^{\text{LDelay}})_{ijk}^{n} + \underline{\Pi}_{\rho,0}^{\text{L}} \bullet (\underline{Q}_{\rho})_{ijk}^{n} + \underline{\Pi}_{\rho,1}^{\text{L}} \bullet (\underline{E})_{ijk}^{n} + \underline{\Pi}_{\rho,2}^{\text{L}} \bullet (\underline{E})_{ijk}^{n+1} \right], \tag{2.56}$$

$$(\underline{Q}_{\rho}^{\text{NLDelay}})_{ijk}^{n+1} = \underline{\Omega_{4}} \bullet \left[(\underline{Q}_{\rho}^{\text{NLDelay}})_{ijk}^{n} + (Q_{\rho}^{\text{NL}})_{ijk}^{n} \underline{\Pi_{\rho,0}^{\text{NL}}} \bullet (\underline{E})_{ijk}^{n} + (Q_{\rho}^{\text{NL}})_{ijk}^{n} \underline{\Pi_{\rho,1}^{\text{NL}}} \bullet (\underline{E})_{ijk}^{n+1} \right] + \underline{\Pi_{\rho,2}^{\text{NL}}} \bullet (\underline{E})_{ijk}^{n} [(\underline{E})_{ijk}^{n} \bullet (\underline{E})_{ijk}^{n}] + \underline{\Pi_{\rho,3}^{\text{NL}}} \bullet (\underline{E})_{ijk}^{n} [(\underline{E})_{ijk}^{n} \bullet (\underline{E})_{ijk}^{n+1}] + \underline{\Pi_{\rho,5}^{\text{NL}}} \bullet (\underline{E})_{ijk}^{n+1} [(\underline{E})_{ijk}^{n} \bullet (\underline{E})_{ijk}^{n+1}] + \underline{\Pi_{\rho,5}^{\text{NL}}} \bullet (\underline{E})_{ijk}^{n+1} [(\underline{E})_{ijk}^{n} \bullet (\underline{E})_{ijk}^{n+1}] + \underline{\Pi_{\rho,6}^{\text{NL}}} \bullet (\underline{E})_{ijk}^{n+1} [(\underline{E})_{ijk}^{n+1} \bullet (\underline{E})_{ijk}^{n+1}] ,$$

$$(2.57)$$

where \underline{S}_{E} and \underline{S}_{H} are given by

$$\underline{S_{E}} = \begin{pmatrix}
\frac{\Delta t}{(\mu_{0}\mu_{R})\Delta y} \left[(E_{z})_{i(j+1/2)k}^{n} - (E_{z})_{i(j-1/2)k}^{n} \right] - \frac{\Delta t}{(\mu_{0}\mu_{R})\Delta z} \left[(E_{y})_{ij(k+1/2)}^{n} - (E_{y})_{ij(k+1/2)}^{n} \right] \\
\frac{\Delta t}{(\mu_{0}\mu_{R})\Delta z} \left[(E_{x})_{ij(k+1/2)}^{n} - (E_{x})_{ij(k-1/2)}^{n} \right] - \frac{\Delta t}{(\mu_{0}\mu_{R})\Delta x} \left[(E_{z})_{(i+1/2)jk}^{n} - (E_{z})_{(i-1/2)jk}^{n} \right] \\
\frac{\Delta t}{(\mu_{0}\mu_{R})\Delta x} \left[(E_{y})_{(i+1/2)jk}^{n} - (E_{y})_{(i-1/2)jk}^{n} \right] - \frac{\Delta t}{(\mu_{0}\mu_{R})\Delta y} \left[(E_{x})_{i(j+1/2)k}^{n} - (E_{x})_{i(j-1/2)k}^{n} \right]$$
(2.58)

$$\underline{S_{H}} = \begin{pmatrix} -\frac{\Delta t}{(\epsilon_{0}\epsilon_{R})\Delta y} \left[(H_{z})_{i(j+\frac{1}{2})k}^{n+\frac{1}{2}} - (H_{z})_{i(j-\frac{1}{2})k}^{n+\frac{1}{2}} \right] + \frac{\Delta t}{(\epsilon_{0}\epsilon_{R})\Delta z} \left[(H_{y})_{ij(k+\frac{1}{2})}^{n+\frac{1}{2}} - (H_{y})_{ij(k-\frac{1}{2})}^{n+\frac{1}{2}} \right] \\ -\frac{\Delta t}{(\epsilon_{0}\epsilon_{R})\Delta z} \left[(H_{x})_{ij(k+\frac{1}{2})}^{n+\frac{1}{2}} - (H_{x})_{ij(k-\frac{1}{2})}^{n+\frac{1}{2}} \right] + \frac{\Delta t}{(\epsilon_{0}\epsilon_{R})\Delta x} \left[(H_{z})_{(i+\frac{1}{2})jk}^{n+\frac{1}{2}} - (H_{z})_{(i-\frac{1}{2})jk}^{n+\frac{1}{2}} \right] \\ -\frac{\Delta t}{(\epsilon_{0}\epsilon_{R})\Delta x} \left[(H_{y})_{(i+\frac{1}{2})jk}^{n+\frac{1}{2}} - (H_{y})_{(i-\frac{1}{2})jk}^{n+\frac{1}{2}} \right] + \frac{\Delta t}{(\epsilon_{0}\epsilon_{R})\Delta y} \left[(H_{x})_{i(j+\frac{1}{2})k}^{n+\frac{1}{2}} - (H_{x})_{i(j-\frac{1}{2})k}^{n+\frac{1}{2}} \right] \end{pmatrix},$$
 (2.59)

and $(\Lambda_0)_{ijk}^n$ and $(\Lambda_1)_{ijk}^n$ are the matrices that depend on $(Q_\rho^{NL})_{ijk}^n$, material properties and Δt , and $\Theta_{\rho,0}^L$, $\Theta_{\rho,1}^L$, $\Theta_{\rho,0}^{NL}$, $\Theta_{\rho,1}^{NL}$, $\Theta_{\rho,2}^{NL}$, Θ

Using the above FDTD-PML algorithm the computer simulation can be performed for electromagnetic waves that propagate inside nonlinear dispersive PML media by simply going through the following steps:

- (1) First, as part of the initial condition, time-invariant coefficients $\Theta_{\rho,0}^L$, $\Theta_{\rho,1}^L$, $\Theta_{\rho,2}^L$, $\Theta_{\rho,0}^{NL}$, $\Theta_{\rho,1}^{NL}$, $\Theta_{\rho,1}^{NL}$, $\Theta_{\rho,2}^{NL}$, and time-invariant matrices Ω_0 , Ω_1 , Ω_2 , Ω_3 , Ω_4 , Ω_5 , Ω_6 , $\Gamma_{\rho,0}^L$, $\Gamma_{\rho,0}^{NL}$, $\Gamma_$
- (2) Using Eq. (2.50), $(\underline{H})_{ijk}^{n+1/2}$ is calculated based on the known values of $(\underline{H})_{ijk}^{n-1/2}$ and $(\underline{H}^{Delay})_{ijk}^{n-1/2}$ and $(\underline{E})_{ijk}^{n}$.
- (3) Using Eq. (2.54), $(\underline{H}^{Delay})_{ijk}^{n+1/2}$ is calculated based on the known values of $(\underline{H}^{Delay})_{ijk}^{n-1/2}$, $(\underline{H})_{ijk}^{n+1/2}$ and $(\underline{H})_{ijk}^{n-1/2}$.
- (4) Using Eqs. (A.8) and (A.12), $(\underline{\Lambda}_0)_{ijk}^n$ and $(\underline{\Lambda}_1)_{ijk}^n$ are calculated, respectively, with the values of $(Q_0^{NL})_{ijk}^n$.
- (5) Using Eq. (2.51), $(\underline{E})_{ijk}^{n+1}$ is calculated based on the known values of $(\underline{E})_{ijk}^{n}$, $(\underline{E}^{Delay})_{ijk}^{n}$, $(Q_{\rho}^{L})_{ijk}^{n}$, $(Q_{\rho}^{L})_{ijk}^{n}$, and $(\underline{H})_{ijk}^{n+1}$. Because Eq. (2.51) represents coupled, cubic, algebraic equations, the nonlinear Newton-Raphson method [11] is used to solve for $(\underline{E})_{ijk}^{n+1}$ by finding the zeroes of Eq. (2.51) with $(\underline{E})_{ijk}^{n}$ as the initial guess.
- (6) Using Eqs. (2.52), (2.53), (2.55), (2.56) and (2.57), $(Q_{\rho}^{L})_{ijk}^{n+1}$, $(Q_{\rho}^{NL})_{ijk}^{n+1}$, $(\underline{E}^{Delay})_{ijk}^{n+1}$, $(\underline{C}_{\rho}^{Delay})_{ijk}^{n+1}$, $(\underline{C}_{\rho}^{Delay})_{ijk}^{n+1}$, $(\underline{E}^{Delay})_{ijk}^{n+1}$, $(\underline{$
- (7) Increment the time step by Δt . Go back to step (2) and repeat the whole process over again. Shown in Figure 1 is the flow chart of numerical steps required to update field values as described above.

In the absence of the PML interface, σ_x , σ_y and σ_z are all set to zeroes and the nonlinear dispersive FDTD-PML algorithm reduces to the usual nonlinear dispersive FDTD algorithm obtained for a nonlinear dispersive medium with the third-order electric susceptibility functions [9,10].

Also, we get the linear FDTD-PML algorithm by simply setting α_{ρ}^{NL} to zero. Furthermore, if both α_{ρ}^{L} and α_{ρ}^{NL} are set to zeroes, the FDTD-PML algorithm reduces to the case of the simple PML algorithm in free space.

III. CONCLUSIONS

We present in this paper the formulation of a three-dimensional FDTD-PML algorithm inside nonlinear dispersive PML media that is used to absorb all outgoing electromagnetic waves within a finite simulation volume to create the notion of infinity at the outer layer boundary of the computational volume. Because of the use of the piecewise-linear approximation, the FDTD-PML algorithm provides second-order accuracy in time for the calculation of electromagnetic field quantities. The resulting forms of the FDTD-PML algorithm tell us that we need to solve coupled cubic equations for the three components of the electric field vector at each time step due to the nonlinear behavior of the third-order electric susceptibility function. In the absence of the nonlinear contribution, the electric field components are no longer coupled and each component of the electric field vector can be updated independently of the other two components.

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APPENDIX

This appendix gives the explicit expressions of coefficients and matrices seen in Eqs. (2.50) through (2.57). The coefficients and matrices shown below are for $\Theta_{\rho,0}^L$, $\Theta_{\rho,1}^L$, $\Theta_{\rho,2}^L$, $\Theta_{\rho,0}^{NL}$, $\Theta_{\rho,1}^{NL}$, $\Theta_{\rho,2}^{NL}$, $\Theta_{\rho,1}^{NL}$, $\Theta_{\rho,2}^{NL}$, $\Theta_{\rho,1}^{NL}$, $\Theta_{\rho,2}^{NL}$, $\Theta_{\rho,1}^{NL}$, $\Theta_{\rho,2}^{NL}$, $\Theta_{\rho,3}^{NL}$, $(\Lambda_0)_{ijk}^n$, $(\Lambda_1)_{ijk}^n$, $(\Lambda_2)_{ijk}^n$, $(\Lambda$

$$\Theta_{0,0}^{L} = \xi_{0,0}^{L}, \tag{A.1}$$

$$\Theta_{\rho,1}^{L} = \frac{\alpha_{\rho}^{L}}{\epsilon_{n}} [\xi_{\rho,1}^{L} - \xi_{\rho,2}^{L}], \tag{A.2}$$

$$\Theta_{\rho,2}^{L} = \frac{\alpha_{\rho}^{L}}{\varepsilon_{p}} \xi_{\rho,2}^{L}, \tag{A.3}$$

$$\Theta_{0,0}^{\text{NL}} = \xi_{0,0}^{\text{NL}},\tag{A.4}$$

$$\Theta_{\rho,1}^{NL} = \frac{\alpha_{\rho}^{NL}}{\epsilon_{R}} \left[\xi_{\rho,1}^{NL} - 2 \xi_{\rho,2}^{NL} + \xi_{\rho,3}^{NL} \right], \tag{A.5}$$

$$\Theta_{\rho,2}^{NL} = \frac{\alpha_{\rho}^{NL}}{\epsilon_{P}} [2 \, \xi_{\rho,2}^{NL} - 2 \xi_{\rho,3}^{NL}], \tag{A.6}$$

$$\Theta_{\rho,3}^{NL} = \frac{\alpha_{\rho}^{NL}}{\epsilon_{\rho}} \xi_{\rho,3}^{NL}, \qquad (A.7)$$

$$(\underline{\Lambda_0})_{ijk}^n = \begin{pmatrix} [(\Lambda_0)_{ijk}^n]_{11} & 0 & 0 \\ 0 & [(\Lambda_0)_{ijk}^n]_{22} & 0 \\ 0 & 0 & [(\Lambda_0)_{ijk}^n]_{33} \end{pmatrix} \text{ with three diagonal elements expressed as}$$
 (A.8)

$$\begin{split} &[(\Lambda_0)_{ijk}^n]_{11} = 1 + [(\frac{\sigma_y}{\epsilon_0 \epsilon_R}) + (\frac{\sigma_z}{\epsilon_0 \epsilon_R}) - (\frac{\sigma_x}{\epsilon_0 \epsilon_R})] \frac{\Delta t}{2} + [(\frac{\sigma_y}{\epsilon_0 \epsilon_R}) - (\frac{\sigma_x}{\epsilon_0 \epsilon_R})] [(\frac{\sigma_z}{\epsilon_0 \epsilon_R}) - (\frac{\sigma_x}{\epsilon_0 \epsilon_R})] (\phi_2)_x \\ &\quad + \frac{1}{\epsilon_R} \, Re \, \Big\{ \sum_{\rho} \alpha_\rho^L \, \xi_{\rho,0}^L \, \xi_{\rho,1}^L \, \Big\} + \frac{1}{\epsilon_R} [(\frac{\sigma_y}{\epsilon_0 \epsilon_R}) + (\frac{\sigma_z}{\epsilon_0 \epsilon_R}) - (\frac{\sigma_x}{\epsilon_0 \epsilon_R})] Re \, \Big\{ \sum_{\rho} \alpha_\rho^L \, \zeta_{\rho,2}^L \, \Big\} \\ &\quad + \frac{1}{\epsilon_R} \, [(\frac{\sigma_y}{\epsilon_0 \epsilon_R}) - (\frac{\sigma_x}{\epsilon_0 \epsilon_R})] [(\frac{\sigma_z}{\epsilon_0 \epsilon_R}) - (\frac{\sigma_x}{\epsilon_0 \epsilon_R})] Re \, \Big\{ \sum_{\rho} \alpha_\rho^L \, (\zeta_{\rho,2}^L)_x \, \Big\} \\ &\quad + \frac{1}{\epsilon_R} \, Re \, \Big\{ \sum_{\rho} \, \xi_{\rho,0}^{NL} \, (Q_\rho^{NL})_{ijk}^n \, \Big\} \\ &\quad + \frac{1}{\epsilon_R} \, [(\frac{\sigma_y}{\epsilon_0 \epsilon_R}) + (\frac{\sigma_z}{\epsilon_0 \epsilon_R}) - (\frac{\sigma_x}{\epsilon_0 \epsilon_R})] Re \, \Big\{ \sum_{\rho} \, \xi_{\rho,2}^{NL} \, (Q_\rho^{NL})_{ijk}^n \, \Big\} \\ &\quad + \frac{1}{\epsilon_R} \, [(\frac{\sigma_y}{\epsilon_0 \epsilon_R}) - (\frac{\sigma_x}{\epsilon_0 \epsilon_R})] [(\frac{\sigma_z}{\epsilon_0 \epsilon_R}) - (\frac{\sigma_x}{\epsilon_0 \epsilon_R})] Re \, \Big\{ \sum_{\rho} \, \xi_{\rho,2}^{NL} \, (Q_\rho^{NL})_{ijk}^n \, \Big\} \, , \end{split} \tag{A.9}$$

$$[(\Lambda_0)_{ijk}^n]_{22} = \text{Replace } [x \rightarrow y, y \rightarrow z, \text{ and } z \rightarrow x] \text{ in } [(\Lambda_0)_{ijk}^n]_{11}, \tag{A.10}$$

$$[(\Lambda_0)_{ijk}^n]_{33} = \text{Replace } [\mathbf{x} \rightarrow \mathbf{z}, \mathbf{y} \rightarrow \mathbf{x}, \text{ and } \mathbf{z} \rightarrow \mathbf{y}] \text{ in } [(\Lambda_0)_{ijk}^n]_{11}, \tag{A.11}$$

$$(\underline{\underline{\Lambda}_1})_{ijk}^n = \begin{pmatrix} [(\Lambda_1)_{ijk}^n]_{11} & 0 & 0 \\ 0 & [(\Lambda_1)_{ijk}^n]_{22} & 0 \\ 0 & 0 & [(\Lambda_1)_{ijk}^n]_{33} \end{pmatrix} \text{ with three diagonal elements expressed as}$$
 (A.12)

$$\begin{split} &[(\Lambda_{1})_{ijk}^{n}]_{11} = -1 + [(\frac{\sigma_{y}}{\epsilon_{0}\epsilon_{R}}) + (\frac{\sigma_{z}}{\epsilon_{0}\epsilon_{R}}) - (\frac{\sigma_{x}}{\epsilon_{0}\epsilon_{R}})] \frac{\Delta t}{2} + [(\frac{\sigma_{y}}{\epsilon_{0}\epsilon_{R}}) - (\frac{\sigma_{x}}{\epsilon_{0}\epsilon_{R}})] [(\frac{\sigma_{z}}{\epsilon_{0}\epsilon_{R}}) - (\frac{\sigma_{x}}{\epsilon_{0}\epsilon_{R}})] [(\phi_{1})_{x} - (\phi_{2})_{x}] \\ &+ \frac{1}{\epsilon_{R}} \operatorname{Re} \left\{ \sum_{\rho} \alpha_{\rho}^{L} \xi_{\rho,0}^{L} [\xi_{\rho,1}^{L} - \xi_{\rho,2}^{L}] \right\} + \frac{1}{\epsilon_{R}} [(\frac{\sigma_{y}}{\epsilon_{0}\epsilon_{R}}) + (\frac{\sigma_{z}}{\epsilon_{0}\epsilon_{R}}) - (\frac{\sigma_{x}}{\epsilon_{0}\epsilon_{R}})] \operatorname{Re} \left\{ \sum_{\rho} \alpha_{\rho}^{L} [\xi_{\rho,1}^{L} - \xi_{\rho,2}^{L}] \right\} \\ &+ \frac{1}{\epsilon_{R}} [(\frac{\sigma_{y}}{\epsilon_{0}\epsilon_{R}}) - (\frac{\sigma_{x}}{\epsilon_{0}\epsilon_{R}})] [(\frac{\sigma_{z}}{\epsilon_{0}\epsilon_{R}}) - (\frac{\sigma_{x}}{\epsilon_{0}\epsilon_{R}})] \operatorname{Re} \left\{ \sum_{\rho} \alpha_{\rho}^{L} [(\xi_{\rho,1}^{L})_{x} - (\xi_{\rho,2}^{L})_{x}] \right\} \\ &- \frac{1}{\epsilon_{R}} \operatorname{Re} \left\{ \sum_{\rho} (Q_{\rho}^{NL})_{ijk}^{n} \right\} + \frac{1}{\epsilon_{R}} [(\frac{\sigma_{y}}{\epsilon_{0}\epsilon_{R}}) + (\frac{\sigma_{z}}{\epsilon_{0}\epsilon_{R}}) - (\frac{\sigma_{x}}{\epsilon_{0}\epsilon_{R}})] \operatorname{Re} \left\{ \sum_{\rho} [\xi_{\rho,1}^{NL} - \xi_{\rho,2}^{NL}] (Q_{\rho}^{NL})_{ijk}^{n} \right\} \\ &+ \frac{1}{\epsilon_{R}} [(\frac{\sigma_{y}}{\epsilon_{0}\epsilon_{R}}) - (\frac{\sigma_{x}}{\epsilon_{0}\epsilon_{R}})] [(\frac{\sigma_{z}}{\epsilon_{0}\epsilon_{R}}) - (\frac{\sigma_{x}}{\epsilon_{0}\epsilon_{R}})] \operatorname{Re} \left\{ \sum_{\rho} \xi_{\rho,1}^{NL} (Q_{\rho}^{NL})_{ijk}^{n} \right\}, \end{split} \tag{A.13}$$

$$[(\Lambda_1)_{ijk}^n]_{22} = \text{Replace } [x \rightarrow y, y \rightarrow z, \text{ and } z \rightarrow x] \text{ in } [(\Lambda_1)_{ijk}^n]_{11}, \tag{A.14}$$

$$[(\Lambda_1)_{ijk}^n]_{33} = \text{Replace } [x \rightarrow z, y \rightarrow x, \text{ and } z \rightarrow y] \text{ in } [(\Lambda_1)_{ijk}^n]_{11}, \tag{A.15}$$

$$\underline{\underline{\Omega_0}} = \begin{pmatrix} (\Omega_0)_{11} & 0 & 0 \\ 0 & (\Omega_0)_{22} & 0 \\ 0 & 0 & (\Omega_0)_{33} \end{pmatrix} \text{ with three diagonal elements expressed as}$$
(A.16)

$$(\Omega_0)_{11} = 1 + \left[\left(\frac{\sigma_y}{\epsilon_0 \epsilon_R} \right) + \left(\frac{\sigma_z}{\epsilon_0 \epsilon_R} \right) - \left(\frac{\sigma_x}{\epsilon_0 \epsilon_R} \right) \right] \frac{\Delta t}{2} + \left[\left(\frac{\sigma_y}{\epsilon_0 \epsilon_R} \right) - \left(\frac{\sigma_x}{\epsilon_0 \epsilon_R} \right) \right] \left(\frac{\sigma_z}{\epsilon_0 \epsilon_R} \right) - \left(\frac{\sigma_x}{\epsilon_0 \epsilon_R} \right) \right] (\phi_2)_x, \tag{A.17}$$

$$(\Omega_0)_{22}$$
 = Replace [x \rightarrow y, y \rightarrow z, and z \rightarrow x] in $(\Omega_0)_{11}$, (A.18)

$$(\Omega_0)_{33}$$
 = Replace [x \rightarrow z, y \rightarrow x, and z \rightarrow y] in $(\Omega_0)_{11}$, (A.19)

$$\underline{\underline{\Omega_1}} = \begin{pmatrix} (\Omega_1)_{11} & 0 & 0 \\ 0 & (\Omega_1)_{22} & 0 \\ 0 & 0 & (\Omega_1)_{33} \end{pmatrix} \text{ with three diagonal elements expressed as}$$
 (A.20)

$$(\Omega_1)_{11} = -1 + [(\frac{\sigma_y}{\epsilon_0 \epsilon_R}) + (\frac{\sigma_z}{\epsilon_0 \epsilon_R}) - (\frac{\sigma_x}{\epsilon_0 \epsilon_R})] \frac{\Delta t}{2} + [(\frac{\sigma_y}{\epsilon_0 \epsilon_R}) - (\frac{\sigma_x}{\epsilon_0 \epsilon_R})] [(\frac{\sigma_z}{\epsilon_0 \epsilon_R}) - (\frac{\sigma_x}{\epsilon_0 \epsilon_R})] [(\phi_1)_x - (\phi_2)_x], (A.21)$$

$$(\Omega_1)_{22}$$
 = Replace $[x \rightarrow y, y \rightarrow z, \text{ and } z \rightarrow x]$ in $(\Omega_1)_{11}$, (A.22)

$$(\Omega_1)_{33}$$
 = Replace [x \rightarrow z, y \rightarrow x, and z \rightarrow y] in $(\Omega_1)_{11}$, (A.23)

$$\underline{\underline{\Omega_2}} = \begin{pmatrix} (\Omega_2)_{11} & 0 & 0 \\ 0 & (\Omega_2)_{22} & 0 \\ 0 & 0 & (\Omega_2)_{33} \end{pmatrix} \text{ with three diagonal elements expressed as}$$
(A.24)

$$(\Omega_2)_{11} = \left[\left(\frac{\sigma_y}{\varepsilon_0 \varepsilon_R} \right) - \left(\frac{\sigma_x}{\varepsilon_0 \varepsilon_R} \right) \right] \left[\left(\frac{\sigma_z}{\varepsilon_0 \varepsilon_R} \right) - \left(\frac{\sigma_x}{\varepsilon_0 \varepsilon_R} \right) \right] (\psi_1)_x, \tag{A.25}$$

$$(\Omega_2)_{22}$$
 = Replace [x \rightarrow y, y \rightarrow z, and z \rightarrow x] in $(\Omega_2)_{11}$, (A.26)

$$(\Omega_2)_{33}$$
 = Replace [x \rightarrow z, y \rightarrow x, and z \rightarrow y] in $(\Omega_2)_{11}$, (A.27)

$$\underline{\underline{\Omega}_{3}} = \begin{pmatrix} \frac{1}{\varepsilon_{R}} (\Omega_{2})_{11} & 0 & 0 \\ 0 & \frac{1}{\varepsilon_{R}} (\Omega_{2})_{22} & 0 \\ 0 & 0 & \frac{1}{\varepsilon_{R}} (\Omega_{2})_{33} \end{pmatrix} \text{ with three diagonal elements expressed as}$$
(A.28)

$$\underline{\underline{\Omega_4}} = \begin{pmatrix} (\psi_0)_x & 0 & 0 \\ 0 & (\psi_0)_y & 0 \\ 0 & 0 & (\psi_0)_z \end{pmatrix}, \tag{A.29}$$

$$\underline{\underline{\Omega_5}} = \begin{pmatrix} [(\psi_1)_x - (\psi_2)_x] & 0 & 0 \\ 0 & [(\psi_1)_y - (\psi_2)_y] & 0 \\ 0 & 0 & [(\psi_1)_z - (\psi_2)_z] \end{pmatrix}, \tag{A.30}$$

$$\underline{\underline{\Omega_6}} = \begin{pmatrix} (\psi_2)_x & 0 & 0 \\ 0 & (\psi_2)_y & 0 \\ 0 & 0 & (\psi_2)_z \end{pmatrix}, \tag{A.31}$$

$$\underline{\Gamma_{\rho,0}^{L}} = \begin{pmatrix} (\Gamma_{\rho,0}^{L})_{11} & 0 & 0 \\ 0 & (\Gamma_{\rho,0}^{L})_{22} & 0 \\ 0 & 0 & (\Gamma_{\rho,0}^{L})_{33} \end{pmatrix} \text{ with three diagonal elements expressed as}$$
(A.32)

$$\begin{split} &(\Gamma_{\rho,0}^{L})_{11} = [\; \xi_{\rho,0}^{L} - 1] + [\; (\frac{\sigma_{y}}{\epsilon_{0}\epsilon_{R}}) + (\frac{\sigma_{z}}{\epsilon_{0}\epsilon_{R}}) - (\frac{\sigma_{x}}{\epsilon_{0}\epsilon_{R}}) \;] \; \xi_{\rho,1}^{L} \\ &+ [(\frac{\sigma_{y}}{\epsilon_{0}\epsilon_{R}}) - (\frac{\sigma_{x}}{\epsilon_{0}\epsilon_{R}})] [(\frac{\sigma_{z}}{\epsilon_{0}\epsilon_{R}}) - (\frac{\sigma_{x}}{\epsilon_{0}\epsilon_{R}})] \; (\zeta_{\rho,0}^{L})_{x} \;, \end{split} \tag{A.33}$$

$$(\Gamma_{\rho,0}^{L})_{22}$$
 = Replace [x \rightarrow y, y \rightarrow z, and z \rightarrow x] in $(\Gamma_{\rho,0}^{L})_{11}$, (A.34)

$$(\Gamma_{\rho,0}^{L})_{33}$$
 = Replace [x \rightarrow z, y \rightarrow x, and z \rightarrow y] in $(\Gamma_{\rho,0}^{L})_{11}$, (A.35)

$$\underline{\underline{\Gamma^{NL}_{\rho,0}}} = \begin{pmatrix} \frac{\alpha^{NL}_{\rho}}{\epsilon_R} (\Gamma^{NL}_{\rho,0})_{11} & 0 & 0 \\ 0 & \frac{\alpha^{NL}_{\rho}}{\epsilon_R} (\Gamma^{NL}_{\rho,0})_{22} & 0 \\ 0 & 0 & \frac{\alpha^{NL}_{\rho}}{\epsilon_R} (\Gamma^{NL}_{\rho,0})_{33} \end{pmatrix} \text{ with three diagonal elements expressed as } (A.36)$$

$$\begin{split} &(\Gamma_{\rho,0}^{NL})_{11} = [\,(\frac{\sigma_{y}}{\epsilon_{0}\epsilon_{R}}) + (\frac{\sigma_{z}}{\epsilon_{0}\epsilon_{R}}) - (\frac{\sigma_{x}}{\epsilon_{0}\epsilon_{R}})\,] \,[\,\,\varsigma_{\rho,1}^{NL} - 3\,\varsigma_{\rho,2}^{NL} + 3\,\varsigma_{\rho,3}^{NL} - \varsigma_{\rho,4}^{NL}\,] \\ &+ [(\frac{\sigma_{y}}{\epsilon_{0}\epsilon_{R}}) - (\frac{\sigma_{x}}{\epsilon_{0}\epsilon_{R}})] [(\frac{\sigma_{z}}{\epsilon_{0}\epsilon_{R}}) - (\frac{\sigma_{x}}{\epsilon_{0}\epsilon_{R}})] [\,\,(\zeta_{\rho,2}^{NL})_{x} - 2\,(\zeta_{\rho,3}^{NL})_{x} + (\zeta_{\rho,4}^{NL})_{x} - (\zeta_{\rho,5}^{NL})_{x} - 2\,(\zeta_{\rho,6}^{NL})_{x} + (\zeta_{\rho,7}^{NL})_{x}\,], \end{split}$$

$$(\Gamma_{\rho,0}^{\text{NL}})_{22} = \text{Replace } [x \rightarrow y, y \rightarrow z, \text{ and } z \rightarrow x] \text{ in } (\Gamma_{\rho,0}^{\text{NL}})_{11},$$
(A.38)

$$(\Gamma_{\rho,0}^{\text{NL}})_{33}$$
 = Replace [x \rightarrow z, y \rightarrow x, and z \rightarrow y] in $(\Gamma_{\rho,0}^{\text{NL}})_{11}$, (A.39)

$$\underline{\underline{\Gamma_{\rho,l}^{NL}}} = \begin{pmatrix}
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$$\begin{split} &(\Gamma_{\rho,1}^{NL})_{11} = [\,(\frac{\sigma_{y}}{\epsilon_{0}\epsilon_{R}}) + (\frac{\sigma_{z}}{\epsilon_{0}\epsilon_{R}}) - (\frac{\sigma_{x}}{\epsilon_{0}\epsilon_{R}})\,][\,2\,\varsigma_{\rho,2}^{NL} - 4\,\varsigma_{\rho,3}^{NL} + 2\,\varsigma_{\rho,4}^{NL}\,] \\ &+ [(\frac{\sigma_{y}}{\epsilon_{0}\epsilon_{R}}) - (\frac{\sigma_{x}}{\epsilon_{0}\epsilon_{R}})][(\frac{\sigma_{z}}{\epsilon_{0}\epsilon_{R}}) - (\frac{\sigma_{x}}{\epsilon_{0}\epsilon_{R}})][\,2\,(\zeta_{\rho,3}^{NL})_{x} - 2\,(\zeta_{\rho,6}^{NL})_{x} - 2\,(\zeta_{\rho,6}^{NL})_{x} + 2\,(\zeta_{\rho,7}^{NL})_{x}\,]\,, \end{split} \tag{A.41}$$

$$(\Gamma_{0,1}^{NL})_{22}$$
 = Replace [x \rightarrow y, y \rightarrow z, and z \rightarrow x] in $(\Gamma_{0,1}^{NL})_{11}$, (A.42)

$$(\Gamma_{\rho,1}^{NL})_{33}$$
 = Replace [x \rightarrow z, y \rightarrow x, and z \rightarrow y] in $(\Gamma_{\rho,1}^{NL})_{11}$, (A.43)

$$\underline{\underline{\Gamma^{NL}_{\rho,2}}} = \begin{pmatrix} \frac{\alpha^{NL}_{\rho}}{\epsilon_R} (\Gamma^{NL}_{\rho,2})_{11} & 0 & 0 \\ 0 & \frac{\alpha^{NL}_{\rho}}{\epsilon_R} (\Gamma^{NL}_{\rho,2})_{22} & 0 \\ 0 & 0 & \frac{\alpha^{NL}_{\rho}}{\epsilon_R} (\Gamma^{NL}_{\rho,2})_{33} \end{pmatrix} \text{ with three diagonal elements expressed as } (A.44)$$

$$\begin{split} &(\Gamma_{\rho,2}^{\rm NL})_{11} = [\,(\frac{\sigma_y}{\epsilon_0 \epsilon_{\rm R}}) + (\frac{\sigma_z}{\epsilon_0 \epsilon_{\rm R}}) - (\frac{\sigma_x}{\epsilon_0 \epsilon_{\rm R}})\,] [\,\varsigma_{\rho,3}^{\rm NL} - \varsigma_{\rho,4}^{\rm NL}\,] \\ &+ [(\frac{\sigma_y}{\epsilon_0 \epsilon_{\rm R}}) - (\frac{\sigma_x}{\epsilon_0 \epsilon_{\rm R}})] [(\frac{\sigma_z}{\epsilon_0 \epsilon_{\rm R}}) - (\frac{\sigma_x}{\epsilon_0 \epsilon_{\rm R}})] [\,(\zeta_{\rho,4}^{\rm NL})_x - (\zeta_{\rho,7}^{\rm NL})_x\,]\,, \end{split} \tag{A.45}$$

$$(\Gamma_{\rho,2}^{\text{NL}})_{22}$$
 = Replace [x \rightarrow y, y \rightarrow z, and z \rightarrow x] in $(\Gamma_{\rho,2}^{\text{NL}})_{11}$, (A.46)

$$(\Gamma_{0,2}^{NL})_{33}$$
 = Replace [x \rightarrow z, y \rightarrow x, and z \rightarrow y] in $(\Gamma_{0,2}^{NL})_{11}$, (A.47)

$$\underline{\underline{\Gamma^{NL}_{\rho,3}}} = \begin{pmatrix} \frac{\alpha^{NL}_{\rho}}{\epsilon_R} (\Gamma^{NL}_{\rho,3})_{11} & 0 & 0 \\ 0 & \frac{\alpha^{NL}_{\rho}}{\epsilon_R} (\Gamma^{NL}_{\rho,3})_{22} & 0 \\ 0 & 0 & \frac{\alpha^{NL}_{\rho}}{\epsilon_R} (\Gamma^{NL}_{\rho,3})_{33} \end{pmatrix} \text{ with three diagonal elements expressed as } (A.48)$$

$$\begin{split} &(\Gamma_{\rho,3}^{\text{NL}})_{11} = \xi_{\rho,0}^{\text{NL}} \left[\xi_{\rho,1}^{\text{NL}} - 2 \, \xi_{\rho,2}^{\text{NL}} + \xi_{\rho,3}^{\text{NL}} \right] + \left[\left(\frac{\sigma_y}{\epsilon_0 \epsilon_R} \right) + \left(\frac{\sigma_z}{\epsilon_0 \epsilon_R} \right) - \left(\frac{\sigma_x}{\epsilon_0 \epsilon_R} \right) \right] \left[\, \zeta_{\rho,2}^{\text{NL}} - 2 \, \zeta_{\rho,3}^{\text{NL}} + \zeta_{\rho,4}^{\text{NL}} \right] \\ &\quad + \left[\left(\frac{\sigma_y}{\epsilon_0 \epsilon_R} \right) - \left(\frac{\sigma_x}{\epsilon_0 \epsilon_R} \right) \right] \left[\left(\frac{\sigma_z}{\epsilon_0 \epsilon_R} \right) - \left(\frac{\sigma_x}{\epsilon_0 \epsilon_R} \right) \right] \left[\left(\zeta_{\rho,5}^{\text{NL}} \right)_x - 2 \left(\zeta_{\rho,6}^{\text{NL}} \right)_x + \left(\zeta_{\rho,7}^{\text{NL}} \right)_x \right], \end{split} \tag{A.49}$$

$$(\Gamma_{\rho,3}^{\text{NL}})_{22} = \text{Replace} [x \rightarrow y, y \rightarrow z, \text{ and } z \rightarrow x] \text{ in } (\Gamma_{\rho,3}^{\text{NL}})_{11},$$
 (A.50)

$$(\Gamma_{\rho,3}^{NL})_{33}$$
 = Replace [x \rightarrow z, y \rightarrow x, and z \rightarrow y] in $(\Gamma_{\rho,3}^{NL})_{11}$, (A.51)

$$\underline{\underline{\Gamma_{\rho,4}^{NL}}} = \begin{pmatrix} \frac{\alpha_{\rho}^{NL}}{\epsilon_R} (\Gamma_{\rho,4}^{NL})_{11} & 0 & 0 \\ 0 & \frac{\alpha_{\rho}^{NL}}{\epsilon_R} (\Gamma_{\rho,4}^{NL})_{22} & 0 \\ 0 & 0 & \frac{\alpha_{\rho}^{NL}}{\epsilon_R} (\Gamma_{\rho,4}^{NL})_{33} \end{pmatrix} \text{ with three diagonal elements expressed as } (A.52)$$

$$\begin{split} &(\Gamma_{\rho,4}^{NL})_{11} = \xi_{\rho,0}^{NL} \left[2 \, \xi_{\rho,2}^{NL} - 2 \xi_{\rho,3}^{NL} \right] + \left[\left(\frac{\sigma_{y}}{\epsilon_{0} \epsilon_{R}} \right) + \left(\frac{\sigma_{z}}{\epsilon_{0} \epsilon_{R}} \right) - \left(\frac{\sigma_{x}}{\epsilon_{0} \epsilon_{R}} \right) \right] \left[2 \, \zeta_{\rho,3}^{NL} - 2 \, \zeta_{\rho,4}^{NL} \right] \\ &+ \left[\left(\frac{\sigma_{y}}{\epsilon_{0} \epsilon_{R}} \right) - \left(\frac{\sigma_{x}}{\epsilon_{0} \epsilon_{R}} \right) \right] \left[\left(\frac{\sigma_{z}}{\epsilon_{0} \epsilon_{R}} \right) - \left(\frac{\sigma_{x}}{\epsilon_{0} \epsilon_{R}} \right) \right] \left[2 \, \left(\zeta_{\rho,6}^{NL} \right)_{x} - 2 \, \left(\zeta_{\rho,7}^{NL} \right)_{x} \right] \,, \end{split} \tag{A.53}$$

$$(\Gamma_{\rho,4}^{NL})_{22}$$
 = Replace [x \rightarrow y, y \rightarrow z, and z \rightarrow x] in $(\Gamma_{\rho,4}^{NL})_{11}$, (A.54)

$$(\Gamma_{0,4}^{\text{NL}})_{33} = \text{Replace} [x \rightarrow z, y \rightarrow x, \text{ and } z \rightarrow y] \text{ in } (\Gamma_{0,4}^{\text{NL}})_{11},$$
(A.55)

$$\underline{\underline{\Gamma_{\rho,5}^{NL}}} = \begin{pmatrix} \frac{\alpha_{\rho}^{NL}}{\epsilon_R} (\Gamma_{\rho,5}^{NL})_{11} & 0 & 0 \\ 0 & \frac{\alpha_{\rho}^{NL}}{\epsilon_R} (\Gamma_{\rho,5}^{NL})_{22} & 0 \\ 0 & 0 & \frac{\alpha_{\rho}^{NL}}{\epsilon_R} (\Gamma_{\rho,5}^{NL})_{33} \end{pmatrix} \text{ with three diagonal elements expressed as } (A.56)$$

$$\begin{split} (\Gamma_{\rho,5}^{NL})_{11} &= \xi_{\rho,0}^{NL} \, \xi_{\rho,3}^{NL} + \left[\left(\frac{\sigma_{y}}{\epsilon_{0} \epsilon_{R}} \right) + \left(\frac{\sigma_{z}}{\epsilon_{0} \epsilon_{R}} \right) - \left(\frac{\sigma_{x}}{\epsilon_{0} \epsilon_{R}} \right) - \left(\gamma_{\rho}^{NL} \right) \right] \zeta_{\rho,4}^{NL} \\ &+ \left[\left(\frac{\sigma_{y}}{\epsilon_{0} \epsilon_{R}} \right) - \left(\frac{\sigma_{x}}{\epsilon_{0} \epsilon_{R}} \right) \right] \left[\left(\frac{\sigma_{z}}{\epsilon_{0} \epsilon_{R}} \right) - \left(\frac{\sigma_{x}}{\epsilon_{0} \epsilon_{R}} \right) \right] \left(\zeta_{\rho,7}^{NL} \right)_{x}, \end{split} \tag{A.57}$$

$$(\Gamma_{0,5}^{\text{NL}})_{22} = \text{Replace} [x \rightarrow y, y \rightarrow z, \text{ and } z \rightarrow x] \text{ in } (\Gamma_{0,5}^{\text{NL}})_{11},$$
(A.58)

$$(\Gamma_{\rho,5}^{NL})_{33}$$
 = Replace [x \rightarrow z, y \rightarrow x, and z \rightarrow y] in $(\Gamma_{\rho,5}^{NL})_{11}$, (A.59)

$$\underline{\underline{\Pi_{\rho,0}^{L}}} = \begin{pmatrix} \frac{\alpha_{\rho}^{L}}{\epsilon_{R}} (\pi_{\rho,0}^{L})_{x} & 0 & 0 \\ 0 & \frac{\alpha_{\rho}^{L}}{\epsilon_{R}} (\pi_{\rho,0}^{L})_{y} & 0 \\ 0 & 0 & \frac{\alpha_{\rho}^{L}}{\epsilon_{R}} (\pi_{\rho,0}^{L})_{z} \end{pmatrix}, \tag{A.60}$$

$$\underline{\underline{\Pi_{\rho,1}^{L}}} = \begin{pmatrix}
\frac{\alpha_{\rho}^{L}}{\epsilon_{R}} [(\pi_{\rho,1}^{L})_{x} - (\pi_{\rho,2}^{L})_{x}] & 0 & 0 \\
0 & \frac{\alpha_{\rho}^{L}}{\epsilon_{R}} [(\pi_{\rho,1}^{L})_{y} - (\pi_{\rho,2}^{L})_{y}] & 0 \\
0 & 0 & \frac{\alpha_{\rho}^{L}}{\epsilon_{R}} [(\pi_{\rho,1}^{L})_{z} - (\pi_{\rho,2}^{L})_{z}]
\end{pmatrix}, (A.61)$$

$$\underline{\underline{\Pi_{\rho,2}^{L}}} = \begin{pmatrix} \underline{\alpha_{\rho}^{L}} (\pi_{\rho,2}^{L})_{x} & 0 & 0 \\ 0 & \underline{\alpha_{\rho}^{L}} (\pi_{\rho,2}^{L})_{y} & 0 \\ 0 & 0 & \underline{\alpha_{\rho}^{L}} (\pi_{\rho,2}^{L})_{z} \end{pmatrix}, \tag{A.62}$$

$$\underline{\underline{\Pi_{\rho,0}^{NL}}} = \begin{pmatrix}
\frac{\alpha_{\rho}^{NL}}{\epsilon_{R}} [(\pi_{\rho,0}^{NL})_{x} - (\pi_{\rho,1}^{NL})_{x}] & 0 & 0 \\
0 & \frac{\alpha_{\rho}^{NL}}{\epsilon_{R}} [(\pi_{\rho,0}^{NL})_{y} - (\pi_{\rho,1}^{NL})_{y}] & 0 \\
0 & 0 & \frac{\alpha_{\rho}^{NL}}{\epsilon_{R}} [(\pi_{\rho,0}^{NL})_{z} - (\pi_{\rho,1}^{NL})_{z}]
\end{pmatrix}, (A.63)$$

$$\underline{\underline{\Pi}_{\rho,1}^{NL}} = \begin{pmatrix} \frac{\alpha_{\rho}^{NL}}{\epsilon_{R}} (\pi_{\rho,1}^{NL})_{x} & 0 & 0 \\ 0 & \frac{\alpha_{\rho}^{NL}}{\epsilon_{R}} (\pi_{\rho,1}^{NL})_{y} & 0 \\ 0 & 0 & \frac{\alpha_{\rho}^{NL}}{\epsilon_{R}} (\pi_{\rho,1}^{NL})_{z} \end{pmatrix}, \tag{A.64}$$

$$\underline{\underline{\Pi_{\rho,2}^{NL}}} = \begin{pmatrix} \frac{\alpha_{\rho}^{NL}}{\epsilon_{R}} (\Pi_{\rho,2}^{NL})_{11} & 0 & 0 \\ 0 & \frac{\alpha_{\rho}^{NL}}{\epsilon_{R}} (\Pi_{\rho,2}^{NL})_{22} & 0 \\ 0 & 0 & \frac{\alpha_{\rho}^{NL}}{\epsilon_{R}} (\Pi_{\rho,2}^{NL})_{33} \end{pmatrix},$$
(A.65)

$$(\Pi_{0,2}^{NL})_{11} = (\pi_{0,2}^{NL})_x - 2(\pi_{0,3}^{NL})_x + (\pi_{0,4}^{NL})_x - (\pi_{0,5}^{NL})_x + 2(\pi_{0,5}^{NL})_x - (\pi_{0,7}^{NL})_x,$$
(A.66)

$$(\Pi_{0,2}^{NL})_{22} = \text{Replace } [x \rightarrow y] \text{ in } (\Pi_{0,2}^{NL})_{11},$$
(A.67)

$$(\Pi_{0,2}^{NL})_{33} = \text{Replace } [x \to z] \text{ in } (\Pi_{0,2}^{NL})_{11},$$
 (A.68)

$$\underline{\underline{\Pi_{\rho,3}^{NL}}} = \begin{pmatrix} \frac{\alpha_{\rho}^{NL}}{\epsilon_{R}} (\Pi_{\rho,3}^{NL})_{11} & 0 & 0 \\ 0 & \frac{\alpha_{\rho}^{NL}}{\epsilon_{R}} (\Pi_{\rho,3}^{NL})_{22} & 0 \\ 0 & 0 & \frac{\alpha_{\rho}^{NL}}{\epsilon_{R}} (\Pi_{\rho,3}^{NL})_{33} \end{pmatrix}, \tag{A.69}$$

$$(\Pi_{0,3}^{NL})_{11} = (\pi_{0,3}^{NL})_{x} - 2(\pi_{0,4}^{NL})_{x} - 2(\pi_{0,6}^{NL})_{x} + (\pi_{0,7}^{NL})_{x}, \tag{A.70}$$

$$(\Pi_{0,3}^{NL})_{22} = \text{Replace } [x \rightarrow y] \text{ in } (\Pi_{0,3}^{NL})_{11},$$
(A.71)

$$(\Pi_{0,3}^{NL})_{33} = \text{Replace } [x \to z] \text{ in } (\Pi_{0,3}^{NL})_{11},$$
(A.72)

$$\underline{\underline{\Pi_{\rho,4}^{NL}}} = \begin{pmatrix} \frac{\alpha_{\rho}^{NL}}{\epsilon_{R}} (\Pi_{\rho,4}^{NL})_{11} & 0 & 0 \\ 0 & \frac{\alpha_{\rho}^{NL}}{\epsilon_{R}} (\Pi_{\rho,4}^{NL})_{22} & 0 \\ 0 & 0 & \frac{\alpha_{\rho}^{NL}}{\epsilon_{R}} (\Pi_{\rho,4}^{NL})_{33} \end{pmatrix}, \tag{A.73}$$

$$(\Pi_{0,4}^{NL})_{11} = (\pi_{0,4}^{NL})_{x} - (\pi_{0,7}^{NL})_{x}, \tag{A.74}$$

$$(\Pi_{\rho,4}^{NL})_{22} = \text{Replace} [x \to y] \text{ in } (\Pi_{\rho,4}^{NL})_{11},$$
(A.75)

$$(\Pi_{\rho,4}^{NL})_{33} = \text{Replace } [x \to z] \text{ in } (\Pi_{\rho,4}^{NL})_{11},$$
 (A.76)

$$\underline{\Pi_{\rho,5}^{NL}} = \begin{pmatrix}
\frac{\alpha_{\rho}^{NL}}{\epsilon_{R}} (\Pi_{\rho,5}^{NL})_{11} & 0 & 0 \\
0 & \frac{\alpha_{\rho}^{NL}}{\epsilon_{R}} (\Pi_{\rho,5}^{NL})_{22} & 0 \\
0 & 0 & \frac{\alpha_{\rho}^{NL}}{\epsilon_{R}} (\Pi_{\rho,5}^{NL})_{33}
\end{pmatrix}, (A.77)$$

$$(\Pi_{\rho,5}^{NL})_{11} = (\pi_{\rho,5}^{NL})_x - 2(\pi_{\rho,6}^{NL})_x + (\pi_{\rho,7}^{NL})_x,$$
(A.78)

$$(\Pi_{0.5}^{NL})_{22} = \text{Replace } [x \rightarrow y] \text{ in } (\Pi_{0.5}^{NL})_{11},$$
 (A.79)

$$(\Pi_{\rho,5}^{NL})_{33} = \text{Replace } [x \to z] \text{ in } (\Pi_{\rho,5}^{NL})_{11},$$
 (A.80)

$$\underline{\underline{\Pi_{\rho,6}^{NL}}} = \begin{pmatrix}
\frac{\alpha_{\rho}^{NL}}{\epsilon_{R}} (\Pi_{\rho,6}^{NL})_{11} & 0 & 0 \\
0 & \frac{\alpha_{\rho}^{NL}}{\epsilon_{R}} (\Pi_{\rho,6}^{NL})_{22} & 0 \\
0 & 0 & \frac{\alpha_{\rho}^{NL}}{\epsilon_{R}} (\Pi_{\rho,6}^{NL})_{33}
\end{pmatrix}, (A.81)$$

$$(\Pi_{\rho,6}^{NL})_{11} = 2 \left(\pi_{\rho,6}^{NL}\right)_{x} - 2 \left(\pi_{\rho,7}^{NL}\right)_{x}, \tag{A.82}$$

$$(\Pi_{\rho,6}^{NL})_{22} = \text{Replace } [x \rightarrow y] \text{ in } (\Pi_{\rho,6}^{NL})_{11},$$
(A.83)

$$(\Pi_{0.6}^{NL})_{33} = \text{Replace } [x \rightarrow z] \text{ in } (\Pi_{0.6}^{NL})_{11},$$
(A.84)

$$\underline{\underline{\Pi_{\rho,7}^{NL}}} = \begin{pmatrix}
\frac{\alpha_{\rho}^{NL}}{\epsilon_{R}} (\pi_{\rho,7}^{NL})_{x} & 0 & 0 \\
0 & \frac{\alpha_{\rho}^{NL}}{\epsilon_{R}} (\pi_{\rho,7}^{NL})_{y} & 0 \\
0 & 0 & \frac{\alpha_{\rho}^{NL}}{\epsilon_{R}} (\pi_{\rho,7}^{NL})_{z}
\end{pmatrix},$$
(A.85)

with elements defined as follows

$$\xi_{\rho,0}^{L} = \exp[-(\gamma_{\rho}^{L})\Delta t], \qquad (A.86)$$

$$\xi_{\rho,1}^{L} \equiv \int_{0}^{\Delta t} d\tau \exp[-(\gamma_{\rho}^{L})\tau] = \Delta t \left[\frac{1 - \exp[-(\gamma_{\rho}^{L})\Delta t]}{(\gamma_{\rho}^{L})\Delta t} \right], \tag{A.87}$$

$$\xi_{\rho,2}^{L} \equiv \int_{0}^{\Delta t} d\tau \left(\frac{\tau}{\Delta t}\right) \exp\left[-(\gamma_{\rho}^{L})\tau\right] = \Delta t \frac{1}{(\gamma_{\rho}^{L})\Delta t} \left[\frac{1 - \exp\left[-(\gamma_{\rho}^{L})\Delta t\right]}{(\gamma_{\rho}^{L})\Delta t} - \exp\left[-(\gamma_{\rho}^{L})\Delta t\right]\right], \tag{A.88}$$

$$\xi_{0,0}^{NL} = \exp[-(\gamma_0^{NL})\Delta t], \qquad (A.89)$$

$$\xi_{\rho,1}^{NL} \equiv \int_{0}^{\Delta t} d\tau \exp[-(\gamma_{\rho}^{NL})\tau] = \Delta t \left[\frac{1 - \exp[-(\gamma_{\rho}^{NL})\Delta t]}{(\gamma_{\rho}^{NL})\Delta t} \right], \tag{A.90}$$

$$\xi_{\rho,2}^{NL} = \int_{0}^{\Delta t} d\tau \left(\frac{\tau}{\Delta t}\right) \exp\left[-(\gamma_{\rho}^{NL})\tau\right] = \Delta t \frac{1}{(\gamma_{\rho}^{NL})\Delta t} \left[\frac{1 - \exp\left[-(\gamma_{\rho}^{NL})\Delta t\right]}{(\gamma_{\rho}^{NL})\Delta t} - \exp\left[-(\gamma_{\rho}^{NL})\Delta t\right]\right], \tag{A.91}$$

$$\begin{split} \xi_{\rho,3}^{NL} &\equiv \int\limits_{0}^{\Delta t} d\tau \, (\frac{\tau}{\Delta t})^2 \, \exp[-(\gamma_{\rho}^{NL})\tau] \\ &= \Delta t \frac{1}{(\gamma_{\rho}^{NL})\Delta t} \bigg[\frac{1}{[(\gamma_{\rho}^{NL})\Delta t]^2} \Big[1 - \exp[-(\gamma_{\rho}^{NL})\Delta t] \Big] - \exp[-(\gamma_{\rho}^{NL})\Delta t] \Big[1 - \frac{2}{[(\gamma_{\rho}^{NL})\Delta t]^2} \Big] \bigg] \,, \end{split} \tag{A.92}$$

$$\varsigma_{\rho,1}^{L} \equiv \int_{0}^{\Delta t} d\tau \int_{0}^{\tau} d\tau' \exp[-(\gamma_{\rho}^{L})(\tau - \tau')] = (\Delta t)^{2} \frac{1}{(\gamma_{\rho}^{L})\Delta t} \left[1 - \frac{1 - \exp[-(\gamma_{\rho}^{L})\Delta t]}{(\gamma_{\rho}^{L})\Delta t}\right], \tag{A.93}$$

$$\varsigma_{\rho,2}^{L} = \int_{0}^{\Delta t} d\tau \int_{0}^{\tau} d\tau' (\frac{\tau'}{\Delta t}) \exp[-(\gamma_{\rho}^{L})(\tau - \tau')] = (\Delta t)^{2} \frac{1}{(\gamma_{\rho}^{L})\Delta t} \left[\frac{1}{2} - \frac{1}{(\gamma_{\rho}^{L})\Delta t} \left[1 - \frac{1 - \exp[-(\gamma_{\rho}^{L})\Delta t]}{(\gamma_{\rho}^{L})\Delta t} \right] \right], \quad (A.94)$$

$$\varsigma_{\rho,1}^{NL} \equiv \int_{0}^{\Delta t} d\tau \int_{0}^{\tau} d\tau' \exp[-(\gamma_{\rho}^{NL})(\tau - \tau')] = (\Delta t)^{2} \frac{1}{(\gamma_{\rho}^{NL})\Delta t} \left[1 - \frac{1 - \exp[-(\gamma_{\rho}^{NL})\Delta t]}{(\gamma_{\rho}^{NL})\Delta t}\right], \tag{A.95}$$

$$\varsigma_{\rho,2}^{NL} = \int_{0}^{\Delta t} d\tau \int_{0}^{\tau} d\tau' \left(\frac{\tau'}{\Delta t}\right) \exp\left[-(\gamma_{\rho}^{NL})(\tau - \tau')\right]
= (\Delta t)^{2} \frac{1}{(\gamma_{\rho}^{NL})\Delta t} \left[\frac{1}{2} - \frac{1}{(\gamma_{\rho}^{NL})\Delta t} \left[1 - \frac{1 - \exp\left[-(\gamma_{\rho}^{NL})\Delta t\right]}{(\gamma_{\rho}^{NL})\Delta t}\right]\right], \tag{A.96}$$

$$\varsigma_{\rho,3}^{NL} = \int_{0}^{\Delta t} d\tau \int_{0}^{\tau} d\tau' \left(\frac{\tau'}{\Delta t}\right)^{2} \exp\left[-(\gamma_{\rho}^{NL})(\tau - \tau')\right]
= (\Delta t)^{2} \frac{1}{(\gamma_{\rho}^{NL})\Delta t} \left[\frac{1}{3} - \frac{1}{(\gamma_{\rho}^{NL})\Delta t} + \frac{2}{[(\gamma_{\rho}^{NL})\Delta t]^{2}} - \frac{2}{[(\gamma_{\rho}^{NL})\Delta t]^{3}} \left[1 - \exp\left[-(\gamma_{\rho}^{NL})\Delta t\right]\right]\right],$$
(A.97)

$$\varsigma_{\rho,4}^{NL} = \int_{0}^{\Delta t} d\tau \int_{0}^{\tau} d\tau' \left(\frac{\tau'}{\Delta t}\right)^{3} \exp\left[-(\gamma_{\rho}^{NL})(\tau - \tau')\right] \\
= (\Delta t)^{2} \frac{1}{(\gamma_{\rho}^{NL})\Delta t} \left[\frac{1}{4} - \frac{1}{(\gamma_{\rho}^{NL})\Delta t} + \frac{3}{[(\gamma_{\rho}^{NL})\Delta t]^{2}} - \frac{6}{[(\gamma_{\rho}^{NL})\Delta t]^{3}} + \frac{6}{[(\gamma_{\rho}^{NL})\Delta t]^{4}} \left[1 - \exp\left[-(\gamma_{\rho}^{NL})\Delta t\right]\right] \right], \tag{A.98}$$

For the x component:

$$(\psi_0)_x \equiv \exp[-(\frac{\sigma_x}{\epsilon_0 \epsilon_R})\Delta t],$$
 (A.99)

$$(\psi_1)_x \equiv \int_0^{\Delta t} d\tau \exp[-(\frac{\sigma_x}{\varepsilon_0 \varepsilon_R})\tau] = \Delta t \left[\frac{1 - \exp[-(\frac{\sigma_x}{\varepsilon_0 \varepsilon_R})\Delta t]}{(\frac{\sigma_x}{\varepsilon_0 \varepsilon_R})\Delta t} \right], \tag{A.100}$$

$$(\psi_2)_x \equiv \int_0^{\Delta t} d\tau \left(\frac{\tau}{\Delta t}\right) \exp\left[-\left(\frac{\sigma_x}{\varepsilon_0 \varepsilon_R}\right) \tau\right] = \Delta t \frac{1}{\left(\frac{\sigma_x}{\varepsilon_0 \varepsilon_R}\right) \Delta t} \left[\frac{1 - \exp\left[-\left(\frac{\sigma_x}{\varepsilon_0 \varepsilon_R}\right) \Delta t\right)\right]}{\left(\frac{\sigma_x}{\varepsilon_0 \varepsilon_R}\right) \Delta t} - \exp\left[-\left(\frac{\sigma_x}{\varepsilon_0 \varepsilon_R}\right) \Delta t\right)\right], \quad (A.101)$$

$$(\phi_{1})_{x} \equiv \int_{0}^{\Delta t} d\tau \int_{0}^{\tau} d\tau' \exp[-(\frac{\sigma_{x}}{\varepsilon_{0}\varepsilon_{R}})(\tau - \tau')] = (\Delta t)^{2} \frac{1}{(\frac{\sigma_{x}}{\varepsilon_{0}\varepsilon_{R}})\Delta t} \left[1 - \frac{1 - \exp[-(\frac{\sigma_{x}}{\varepsilon_{0}\varepsilon_{R}})\Delta t]}{(\frac{\sigma_{x}}{\varepsilon_{0}\varepsilon_{R}})\Delta t}\right], \tag{A.102}$$

$$(\varphi_2)_x \equiv \int_0^{\Delta t} d\tau \int_0^{\tau} d\tau' (\frac{\tau'}{\Delta t}) \exp[-(\frac{\sigma_x}{\epsilon_0 \epsilon_R})(\tau - \tau')]$$

$$= (\Delta t)^{2} \frac{1}{(\frac{\sigma_{x}}{\varepsilon_{0}\varepsilon_{R}})\Delta t} \left[\frac{1}{2} - \frac{1}{(\frac{\sigma_{x}}{\varepsilon_{0}\varepsilon_{R}})\Delta t} \left[1 - \frac{1 - \exp[-(\frac{\sigma_{x}}{\varepsilon_{0}\varepsilon_{R}})\Delta t]}{(\frac{\sigma_{x}}{\varepsilon_{0}\varepsilon_{R}})\Delta t} \right] \right], \tag{A.103}$$

$$(\zeta_{\rho,0}^{L})_{x} = \int_{0}^{\Delta t} d\tau \int_{0}^{\tau} d\tau' \exp[-(\gamma_{\rho}^{L})\tau'] \exp[-(\frac{\sigma_{x}}{\varepsilon_{0}\varepsilon_{R}})(\tau - \tau')]$$

$$= (\Delta t)^{2} \frac{1}{[(\frac{\sigma_{x}}{\varepsilon_{0}\varepsilon_{R}}) - (\gamma_{\rho}^{L})]\Delta t} \left[\frac{1 - \exp[-(\gamma_{\rho}^{L})\Delta t]}{(\gamma_{\rho}^{L})\Delta t} - \frac{1 - \exp[-(\frac{\sigma_{x}}{\varepsilon_{0}\varepsilon_{R}})\Delta t]}{(\frac{\sigma_{x}}{\varepsilon_{0}\varepsilon_{R}})\Delta t}\right], \tag{A.104}$$

$$\Delta t = \tau - \tau'$$

$$\begin{split} (\zeta_{\rho,l}^{L})_{x} &\equiv \int_{0}^{\Delta t} d\tau \int_{0}^{\tau} d\tau' \int_{0}^{\tau'} d\tau'' & \exp[-(\gamma_{\rho}^{L})(\tau'-\tau'')] \exp[-(\frac{\sigma_{x}}{\epsilon_{0}\epsilon_{R}})(\tau-\tau')] \\ &= (\Delta t)^{3} \frac{1}{(\gamma_{\rho}^{L})\Delta t} \left\{ \left[\frac{1}{(\frac{\sigma_{x}}{\epsilon_{0}\epsilon_{R}})\Delta t} \right] \left[1 - \frac{1 - \exp[-(\frac{\sigma_{x}}{\epsilon_{0}\epsilon_{R}})\Delta t]}{(\frac{\sigma_{x}}{\epsilon_{0}\epsilon_{R}})\Delta t} \right] \right. \\ &\left. - \left[\frac{1}{(\frac{\sigma_{x}}{\epsilon_{0}})\Delta t - (\gamma_{\rho}^{L})\Delta t} \right] \left[\frac{1 - \exp[-(\gamma_{\rho}^{L})\Delta t]}{(\gamma_{\rho}^{L})\Delta t} - \frac{1 - \exp[-(\frac{\sigma_{x}}{\epsilon_{0}\epsilon_{R}})\Delta t]}{(\frac{\sigma_{x}}{\epsilon_{0}\epsilon_{R}})\Delta t} \right] \right\}, \end{split}$$
 (A.105)

$$\begin{split} (\zeta_{\rho,2}^{L})_{x} &\equiv \int_{0}^{\Delta t} d\tau \int_{0}^{\tau} d\tau' \frac{\tau''}{\Delta t} \exp[-(\gamma_{\rho}^{L})(\tau'-\tau'')] \exp[-(\frac{\sigma_{x}}{\epsilon_{0}\epsilon_{R}})(\tau-\tau')] \\ &= (\Delta t)^{3} \frac{1}{(\gamma_{\rho}^{L})\Delta t} \left\{ \left[\frac{1}{(\frac{\sigma_{x}}{\epsilon_{0}\epsilon_{R}})\Delta t} \right] \left[\frac{1}{2} - \left[1 - \frac{1 - \exp[-(\frac{\sigma_{x}}{\epsilon_{0}\epsilon_{R}})\Delta t}] \left[\frac{1}{(\frac{\sigma_{x}}{\epsilon_{0}\epsilon_{R}})\Delta t} + \frac{1}{(\gamma_{\rho}^{L})\Delta t} \right] \right] \right. \\ &+ \left[\frac{1}{(\frac{\sigma_{x}}{\epsilon_{0}\epsilon_{R}})\Delta t} - (\gamma_{\rho}^{L})\Delta t} \right] \left[\frac{1}{(\gamma_{\rho}^{L})\Delta t} \right] \left[\frac{1 - \exp[-(\gamma_{\rho}^{L})\Delta t}]}{(\gamma_{\rho}^{L})\Delta t} - \frac{1 - \exp[-(\frac{\sigma_{x}}{\epsilon_{0}\epsilon_{R}})\Delta t}]}{(\frac{\sigma_{x}}{\epsilon_{0}\epsilon_{R}})\Delta t}} \right] \right\}, \quad (A.106) \end{split}$$

$$\begin{split} &(\zeta_{\rho,0}^{NL})_x \equiv \int\limits_0^{\Delta t} d\tau \int\limits_0^{\tau} d\tau' \exp[-(\gamma_{\rho}^{NL})\tau'] \exp[-(\frac{\sigma_x}{\epsilon_0 \epsilon_R})(\tau - \tau')] \\ &= (\Delta t)^2 \frac{1}{[(\frac{\sigma_x}{\epsilon_0 \epsilon_R})\Delta t - (\gamma_{\rho}^{NL})\Delta t]} \left[\frac{1 - \exp[-(\gamma_{\rho}^{NL})\Delta t]}{(\gamma_{\rho}^{NL})\Delta t} - \frac{1 - \exp[-(\frac{\sigma_x}{\epsilon_0 \epsilon_R})\Delta t]}{(\frac{\sigma_x}{\epsilon_0 \epsilon_R})\Delta t}\right], \end{split} \tag{A.107}$$

$$\begin{split} & (\zeta_{\rho,1}^{NL})_x \equiv \int\limits_0^{\Delta t} d\tau \int\limits_0^\tau d\tau' (\frac{\tau'}{\Delta t}) \exp[-(\gamma_\rho^{NL})\tau'] \exp[-(\frac{\sigma_x}{\epsilon_\rho \epsilon_R})(\tau-\tau')] \\ & = (\Delta t)^2 \frac{1}{(\frac{\sigma_x}{\epsilon_\rho \epsilon_R})\Delta t - (\gamma_\rho^{NL})\Delta t} \bigg\{ \bigg[1 - \exp[-(\gamma_\rho^{NL})\Delta t] \bigg] \frac{1}{[(\gamma_\rho^{NL})\Delta t]^2} \\ & - \bigg[1 - \exp[-(\gamma_\rho^{NL})\Delta t] \bigg] \bigg[\frac{1}{[(\gamma_\rho^{NL})\Delta t]((\frac{\sigma_x}{\epsilon_\rho \epsilon_R})\Delta t - (\gamma_\rho^{NL})\Delta t]} \bigg] \\ & - \frac{\exp[-(\gamma_\rho^{NL})\Delta t]}{(\gamma_\rho^{NL})\Delta t} + \bigg[1 - \exp[-(\frac{\sigma_x}{\epsilon_\rho \epsilon_R})\Delta t] \bigg] \bigg[\frac{1}{[(\frac{\sigma_x}{\epsilon_\rho \epsilon_R})\Delta t - (\gamma_\rho^{NL})\Delta t]} \bigg] \bigg\}, \quad (A.108) \\ & (\zeta_{\rho,2}^{NL})_x \equiv \int\limits_0^{\Delta t} d\tau \int\limits_0^\tau d\tau' \int\limits_0^\tau d\tau'' \exp[-(\gamma_\rho^{NL})(\tau'-\tau'')] \exp[-(\frac{\sigma_x}{\epsilon_\rho \epsilon_R})(\tau-\tau')] \\ & = (\Delta t)^3 \frac{1}{(\gamma_\rho^{NL})\Delta t} \bigg\{ \bigg[\frac{1}{(\frac{\sigma_x}{\epsilon_\rho \epsilon_R})\Delta t} \bigg] \bigg[1 - \frac{1 - \exp[-(\frac{\sigma_x}{\epsilon_\rho \epsilon_R})\Delta t]}{(\frac{\sigma_x}{\epsilon_\rho \epsilon_R})\Delta t} \bigg] \\ & - \bigg[\frac{1}{(\frac{\sigma_x}{\epsilon_\rho \epsilon_R})\Delta t} - (\gamma_\rho^{NL})\Delta t \bigg] \bigg[\frac{1 - \exp[-(\gamma_\rho^{NL})\Delta t]}{(\gamma_\rho^{NL})\Delta t} - \frac{1 - \exp[-(\frac{\sigma_x}{\epsilon_\rho \epsilon_R})\Delta t]}{(\frac{\sigma_x}{\epsilon_\rho \epsilon_R})\Delta t} \bigg] \bigg\}, \quad (A.109) \\ & (\zeta_{\rho,3}^{NL})_x \equiv \int\limits_0^\Delta d\tau \int\limits_0^\tau d\tau' \int\limits_0^\tau d\tau'' \frac{\tau''}{\Delta t} \cdot \exp[-(\gamma_\rho)(\tau'-\tau'')] \exp[-(\frac{\sigma_x}{\epsilon_\rho \epsilon_R})\Delta t] \bigg[\frac{1}{(\frac{\sigma_x}{\epsilon_\rho \epsilon_R})\Delta t} - \frac{1 - \exp[-(\frac{\sigma_x}{\epsilon_\rho \epsilon_R})\Delta t]}{(\frac{\sigma_x}{\epsilon_\rho \epsilon_R})\Delta t} - \frac{1 - \exp[-(\frac{\sigma_x}{\epsilon_\rho \epsilon_R})\Delta t]}{(\frac{\sigma_x}{\epsilon_\rho \epsilon_R})\Delta t} \bigg] \bigg\}, \quad (A.109) \\ & + \bigg[\frac{1}{(\frac{\sigma_x}{\epsilon_\rho \epsilon_R})\Delta t - (\gamma_\rho^{NL})\Delta t} \bigg] \bigg[\frac{1}{(\gamma_\rho^{NL})\Delta t} \bigg] \bigg[\frac{1 - \exp[-(\frac{\sigma_x}{\epsilon_\rho \epsilon_R})\Delta t]}{(\gamma_\rho^{NL})\Delta t} - \frac{1 - \exp[-(\frac{\sigma_x}{\epsilon_\rho \epsilon_R})\Delta t]}{(\frac{\sigma_x}{\epsilon_\rho \epsilon_R})\Delta t} \bigg] \bigg\}, \quad (A.110) \end{aligned}$$

$$\begin{split} &\langle \zeta_{\rho,D}^{NL} \rangle_x \equiv \int\limits_0^{\Delta t} d\tau \int\limits_0^t d\tau' \int\limits_0^{\tau} d\tau' \int\limits_0^{\tau} d\tau' \int\limits_{\epsilon \in E_t}^{\tau} \rangle \exp[-(\gamma_\rho^{NL})(\tau^-\tau^*)] \exp[-(\frac{\sigma_x}{\epsilon \varepsilon E_t})(\tau^-\tau')] \\ &= (\Delta t)^3 \frac{1}{[(\gamma_\rho^{NL})\Delta t][(\frac{\sigma_x}{\epsilon \varepsilon E_t})\Delta t]} \left\{ \frac{1}{3} - \frac{1}{(\frac{\sigma_x}{\epsilon \varepsilon E_t})\Delta t} + \frac{2}{[(\frac{\sigma_x}{\epsilon \varepsilon E_t})\Delta t]^2} - \frac{1}{2(\gamma_\rho^{NL})\Delta t} + \frac{1}{[(\gamma_\rho^{NL})\Delta t][(\frac{\sigma_x}{\epsilon \varepsilon E_t})\Delta t]^2} - \frac{1}{2(\gamma_\rho^{NL})\Delta t]} \right\} \\ &- \left[1 - \exp[-(\frac{\sigma_x}{\epsilon \varepsilon E_t})\Delta t] \right] \left[\frac{2}{[(\frac{\sigma_x}{\epsilon \varepsilon E_t})\Delta t]^3} + \frac{1}{[(\gamma_\rho^{NL})\Delta t][(\frac{\sigma_x}{\epsilon \varepsilon E_t})\Delta t]^2} - \frac{1}{[(\gamma_\rho^{NL})\Delta t][(\frac{\sigma_x}{\epsilon \varepsilon E_t})\Delta t]} \right] \\ &- \left[1 - \exp[-(\gamma_\rho^{NL})\Delta t] \right] \left[\frac{(\frac{\sigma_x}{\epsilon \varepsilon E_t})\Delta t}{[(\gamma_\rho^{NL})\Delta t]^2((\frac{\sigma_x}{\epsilon \varepsilon E_t})\Delta t - (\gamma_\rho^{NL})\Delta t]^2} \right] \\ &- \exp[-(\gamma_\rho^{NL})\Delta t] \left[1 + \frac{1}{(\gamma_\rho^{NL})\Delta t} \right] \left[\frac{(\frac{\sigma_x}{\epsilon \varepsilon E_t})\Delta t}{[(\gamma_\rho^{NL})\Delta t]^2((\frac{\sigma_x}{\epsilon \varepsilon E_t})\Delta t - (\gamma_\rho^{NL})\Delta t]^2} \right] \\ &- \exp[-(\gamma_\rho^{NL})\Delta t] \left[1 + \frac{1}{(\gamma_\rho^{NL})\Delta t} \right] \left[\frac{(\frac{\sigma_x}{\epsilon \varepsilon E_t})\Delta t}{[(\gamma_\rho^{NL})\Delta t]^2((\frac{\sigma_x}{\epsilon \varepsilon E_t})\Delta t - (\gamma_\rho^{NL})\Delta t]^2} \right] \\ &- \exp[-(\gamma_\rho^{NL})\Delta t] \left[\frac{1}{(\gamma_\rho^{NL})\Delta t} \right] \left[\frac{(\frac{\sigma_x}{\epsilon \varepsilon E_t})\Delta t}{[(\gamma_\rho^{NL})\Delta t]^3((\frac{\sigma_x}{\epsilon \varepsilon E_t})\Delta t - (\gamma_\rho^{NL})\Delta t]^3} \right] \\ &- \frac{2}{3(\gamma_\rho^{NL})\Delta t} \frac{1}{[(\gamma_\rho^{NL})\Delta t][(\frac{\sigma_x}{\epsilon \varepsilon E_t})\Delta t]} \left[\frac{1}{(\gamma_\rho^{NL})\Delta t} \right] \frac{(\gamma_\rho^{NL})\Delta t}{[(\gamma_\rho^{NL})\Delta t]^2((\frac{\sigma_x}{\epsilon \varepsilon E_t})\Delta t - (\gamma_\rho^{NL})\Delta t]^3} \right] \\ &+ \left[1 - \exp[-(\gamma_\rho^{NL})\Delta t] \right] \left[\frac{6}{((\gamma_\rho^{NL})\Delta t)^3} \right] \frac{2((\frac{\sigma_x}{\epsilon \varepsilon E_t})\Delta t}{[(\gamma_\rho^{NL})\Delta t]^3((\frac{\sigma_x}{\epsilon \varepsilon E_t})\Delta t - (\gamma_\rho^{NL})\Delta t]^2} \right] \\ &+ \exp[-(\gamma_\rho^{NL})\Delta t] \left[1 + \frac{1}{(\gamma_\rho^{NL})\Delta t} \right] \left[\frac{2((\frac{\sigma_x}{\epsilon \varepsilon E_t})\Delta t})\Delta t - (\gamma_\rho^{NL})\Delta t}{[(\gamma_\rho^{NL})\Delta t]^3((\frac{\sigma_x}{\epsilon \varepsilon E_t})\Delta t - (\gamma_\rho^{NL})\Delta t})^2} \right] \\ &+ \exp[-(\gamma_\rho^{NL})\Delta t] \left[1 + \frac{1}{(\gamma_\rho^{NL})\Delta t} \right] \left[\frac{2((\frac{\sigma_x}{\epsilon \varepsilon E_t})\Delta t})\Delta t - (\gamma_\rho^{NL})\Delta t}{[(\gamma_\rho^{NL})\Delta t]^3((\frac{\sigma_x}{\epsilon \varepsilon E_t})\Delta t - (\gamma_\rho^{NL})\Delta t})^2} \right] \\ &+ \exp[-(\gamma_\rho^{NL})\Delta t] \left[1 + \frac{1}{(\gamma_\rho^{NL})\Delta t} \right] \left[\frac{2((\frac{\sigma_x}{\epsilon \varepsilon E_t})\Delta t})\Delta t - (\gamma_\rho^{NL})\Delta t}{[(\frac{\sigma_x}{\epsilon \varepsilon E_t})\Delta t - (\gamma_\rho^{NL})\Delta t}]^2} \right] \\ &+ \exp[-(\gamma_\rho^{NL})\Delta t] \left[\frac{1}{(\gamma_\rho^{NL})\Delta t} \right] \left[\frac{2((\frac{\sigma_x}{\epsilon \varepsilon E_t})\Delta t})\Delta t - (\gamma_\rho^{NL})\Delta t}{[(\frac{\sigma_x}{\epsilon \varepsilon E_t})\Delta t - (\gamma_\rho^{NL})\Delta t}]^2} \right] \\ &$$

$$(\pi_{\rho,0}^{L})_{x} \equiv \int_{0}^{\Delta t} d\tau \exp[-(\gamma_{\rho}^{L})\tau] \exp[(\frac{\sigma_{x}}{\varepsilon_{0}\varepsilon_{R}})\tau]$$

$$= \Delta t \exp[(\frac{\sigma_{x}}{\varepsilon_{0}\varepsilon_{R}})\Delta t] \left[\frac{\exp[-(\gamma_{\rho}^{L})\Delta t] - \exp[-(\frac{\sigma_{x}}{\varepsilon_{0}\varepsilon_{R}})\Delta t]}{(\frac{\sigma_{x}}{\varepsilon_{0}\varepsilon_{R}})\Delta t - (\gamma_{\rho}^{L})\Delta t} \right], \tag{A.115}$$

$$\begin{split} (\pi_{\rho,l}^L)_x & \equiv \int\limits_0^{\Delta t} d\tau \int\limits_0^\tau d\tau' exp[-(\gamma_\rho^L)(\tau-\tau')] \, exp[(\frac{\sigma_x}{\epsilon_0 \epsilon_R})\tau] \\ & = (\Delta t)^2 \, \frac{exp[(\frac{\sigma_x}{\epsilon_0 \epsilon_R})\Delta t]}{(\gamma_\rho^L)\Delta t} \bigg\{ \left[\frac{1 - exp[-(\frac{\sigma_x}{\epsilon_0 \epsilon_R})\Delta t]}{(\frac{\sigma_x}{\epsilon_0 \epsilon_R})\Delta t} \right] - \left[\frac{exp[-(\gamma_\rho^L)\Delta\,t] - exp[-(\frac{\sigma_x}{\epsilon_0 \epsilon_R})\Delta t] - \left[\frac{\sigma_x}{\epsilon_0 \epsilon_R} \right] \right] \bigg\}, (A.116) \end{split}$$

$$\begin{split} (\pi_{\rho,2}^{L})_{x} &\equiv \int_{0}^{\Delta t} d\tau' (\frac{\tau'}{\Delta t}) \exp[-(\gamma_{\rho}^{L})(\tau - \tau')] \exp[(\frac{\sigma_{x}}{\epsilon_{0}\epsilon_{R}})\tau] \\ &= (\Delta t)^{2} \frac{\exp[(\frac{\sigma_{x}}{\epsilon_{0}\epsilon_{R}})\Delta t]}{[(\frac{\sigma_{x}}{\epsilon_{0}\epsilon_{R}})\Delta t][(\gamma_{\rho}^{L})\Delta t]} \left\{ 1 - \left[\frac{1 - \exp[-(\frac{\sigma_{x}}{\epsilon_{0}\epsilon_{R}})\Delta t]}{(\frac{\sigma_{x}}{\epsilon_{0}\epsilon_{R}})\Delta t} \right] \left[1 + \frac{(\frac{\sigma_{x}}{\epsilon_{0}\epsilon_{R}})\Delta}{(\gamma_{\rho}^{L})\Delta t} \right] \\ &- \left[\frac{\exp[-(\gamma_{\rho}^{L})\Delta t] - \exp[-(\frac{\sigma_{x}}{\epsilon_{0}\epsilon_{R}})\Delta t]}{(\frac{\sigma_{x}}{\epsilon_{0}\epsilon_{R}})\Delta t} \right] \left[\frac{(\frac{\sigma_{x}}{\epsilon_{0}\epsilon_{R}})\Delta t}{(\gamma_{\rho}^{L})\Delta t} \right] \right\}, \end{split} \tag{A.117}$$

$$(\pi_{\rho,0}^{NL})_{x} \equiv \int_{0}^{\Delta t} d\tau \exp[-(\gamma_{\rho}^{NL})\tau] \exp[(\frac{\sigma_{x}}{\varepsilon_{0}\varepsilon_{R}})\tau]$$

$$= \Delta t \exp[(\frac{\sigma_{x}}{\varepsilon_{0}\varepsilon_{R}})\Delta t] \left[\frac{\exp[-(\gamma_{\rho}^{NL})\Delta t] - \exp[-(\frac{\sigma_{x}}{\varepsilon_{0}\varepsilon_{R}})\Delta t]}{(\frac{\sigma_{x}}{\varepsilon_{0}\varepsilon_{R}})\Delta t - (\gamma_{\rho}^{NL})\Delta t} \right], \tag{A.118}$$

$$\begin{split} (\pi_{\rho,1}^{NL})_x &\equiv \int\limits_0^{\Delta t} d\tau \, \tau \exp[-(\gamma_\rho^{NL})\tau] \exp[(\frac{\sigma_x}{\epsilon_0 \epsilon_R})(\tau)] \\ &= (\Delta t)^2 \, \frac{\exp[(\frac{\sigma_x}{\epsilon_0 \epsilon_R})\Delta t]}{(\frac{\sigma_x}{\epsilon_0 \epsilon_R})\Delta t - (\gamma_\rho^{NL})\Delta t} \bigg[\exp[-(\gamma_\rho^{NL})\Delta t] - \frac{\exp[-(\gamma_\rho^{NL})\Delta t] - \exp[-(\frac{\sigma_x}{\epsilon_0 \epsilon_R})\Delta t]}{(\frac{\sigma_x}{\epsilon_0 \epsilon_R})\Delta t - (\gamma_\rho^{NL})\Delta t} \bigg], \end{split} \tag{A.119}$$

$$\begin{split} (\pi_{\rho,2}^{\text{NL}})_{x} &\equiv \int_{0}^{\Delta t} d\tau \int_{0}^{\tau} d\tau' \exp[-(\gamma_{\rho}^{\text{NL}})(\tau - \tau')] \exp[(\frac{\sigma_{x}}{\epsilon_{0}\epsilon_{R}})\tau] \\ &= (\Delta t)^{2} \frac{\exp[(\frac{\sigma_{x}}{\epsilon_{0}\epsilon_{R}})\Delta t]}{(\gamma_{\rho}^{\text{NL}})\Delta t} \Big\{ \left[\frac{1 - \exp[-(\frac{\sigma_{x}}{\epsilon_{0}\epsilon_{R}})\Delta t]}{(\frac{\sigma_{x}}{\epsilon_{0}\epsilon_{R}})\Delta t} \right] \\ &- \left[\frac{\exp[-(\gamma_{\rho}^{\text{NL}})\Delta t] - \exp[-(\frac{\sigma_{x}}{\epsilon_{0}\epsilon_{R}})\Delta t] - \left[\frac{\sigma_{x}}{\epsilon_{0}\epsilon_{R}} \right] \Big\} , \end{split}$$

$$(A.120)$$

$$\begin{split} (\pi_{\rho,3}^{\text{NL}})_{x} &\equiv \int_{0}^{\Delta t} d\tau \int_{0}^{\tau} d\tau' (\frac{\tau'}{\Delta t}) \exp[-(\gamma_{\rho}^{\text{NL}})(\tau - \tau')] \exp[(\frac{\sigma_{x}}{\epsilon_{0}\epsilon_{R}})\tau] \\ &= (\Delta t)^{2} \frac{\exp[(\frac{\sigma_{x}}{\epsilon_{0}\epsilon_{R}})\Delta t]}{[(\frac{\sigma_{x}}{\epsilon_{0}\epsilon_{R}})\Delta t][(\gamma_{\rho}^{\text{NL}})\Delta t]} \left\{ 1 - \left[\frac{1 - \exp[-(\frac{\sigma_{x}}{\epsilon_{0}\epsilon_{R}})\Delta t]}{(\frac{\sigma_{x}}{\epsilon_{0}\epsilon_{R}})\Delta t} \right] \left[1 + \frac{(\frac{\sigma_{x}}{\epsilon_{0}\epsilon_{R}})\Delta}{(\gamma_{\rho}^{\text{NL}})\Delta t} \right] \right. \\ &\left. - \left[\frac{\exp[-(\gamma_{\rho}^{\text{NL}})\Delta t] - \exp[-(\frac{\sigma_{x}}{\epsilon_{0}\epsilon_{R}})\Delta t]}{(\frac{\sigma_{x}}{\epsilon_{0}\epsilon_{R}})\Delta t} \right] \left[\frac{(\frac{\sigma_{x}}{\epsilon_{0}\epsilon_{R}})\Delta t}{(\gamma_{\rho}^{\text{NL}})\Delta t} \right] \right\}, \end{split}$$

$$(A.121)$$

$$\begin{split} (\pi_{\rho,4}^{NL})_x &\equiv \int\limits_0^{\Delta t} d\tau \int\limits_0^\tau d\tau' (\frac{\tau'}{\Delta t})^2 \exp[-(\gamma_\rho^{NL})(\tau-\tau')] \exp[(\frac{\sigma_x}{\epsilon_0 \epsilon_R})\tau] \\ &= (\Delta t)^2 \frac{\exp[(\frac{\sigma_x}{\epsilon_0 \epsilon_R})\Delta t]}{[(\frac{\sigma_x}{\epsilon_0 \epsilon_R})\Delta t][(\gamma_\rho^{NL})\Delta t]} \bigg\{ 1 - \frac{2}{(\frac{\sigma_x}{\epsilon_0 \epsilon_R})\Delta t} - \frac{2}{(\gamma_\rho^{NL})\Delta t} \\ &+ \bigg[1 - \exp[-(\frac{\sigma_x}{\epsilon_0 \epsilon_R})\Delta t] \bigg] \bigg[\frac{2}{[(\frac{\sigma_x}{\epsilon_0 \epsilon_R})\Delta t]^2} + \frac{2}{[(\gamma_\rho^{NL})\Delta t][(\frac{\sigma_x}{\epsilon_0 \epsilon_R})\Delta t]} + \frac{2}{[(\gamma_\rho^{NL})\Delta t]^2} \bigg] \\ &- \bigg[\frac{2[(\frac{\sigma_x}{\epsilon_0 \epsilon_R})\Delta t]}{[(\gamma_\rho^{NL})\Delta t]^2[(\frac{\sigma_x}{\epsilon_0 \epsilon_R})\Delta t]} - [(\gamma_\rho^{NL})\Delta t] \bigg] \bigg[\exp[-(\gamma_\rho^{NL})\Delta t] - \exp[-(\frac{\sigma_x}{\epsilon_0 \epsilon_R})\Delta t] \bigg] \bigg\}, \quad (A.122) \end{split}$$

$$\begin{split} (\pi_{\rho,5}^{NL})_x &\equiv \int\limits_0^\infty d\tau \int\limits_0^\tau d\tau' \cdot \frac{\tau}{\Delta t} \cdot \exp[-(\gamma_\rho^{NL})(\tau-\tau')] \exp[(\frac{\sigma_x}{\epsilon_o \epsilon_n})\tau] \\ &= (\Delta t)^2 \frac{\exp[(\frac{\sigma_x}{\epsilon_o \epsilon_n})\Delta t]}{[(\frac{\sigma_x}{\epsilon_o \epsilon_n})\Delta t][(\gamma_\rho^{NL})\Delta t]} \bigg\{ 1 - \bigg[1 - \exp[-(\frac{\sigma_x}{\epsilon_o \epsilon_n})\Delta t] \bigg] \bigg[\frac{1}{(\frac{\sigma_x}{\epsilon_o \epsilon_n})\Delta t} \bigg] \\ &+ \bigg[\frac{(\frac{\sigma_x}{\epsilon_o \epsilon_n})\Delta t}{[(\frac{\sigma_x}{\epsilon_o \epsilon_n})\Delta t - (\gamma_\rho^{NL})\Delta t]^2} \bigg] \bigg[\exp[-(\gamma_\rho^{NL})\Delta t] - \exp[-(\frac{\sigma_x}{\epsilon_o \epsilon_n})\Delta t] \bigg] \\ &- \bigg[\frac{(\frac{\sigma_x}{\epsilon_o \epsilon_n})\Delta t}{(\frac{\sigma_x}{\epsilon_o \epsilon_n})\Delta t - (\gamma_\rho^{NL})\Delta t} \bigg] \bigg[\exp[-(\gamma_\rho^{NL})\Delta t] - \exp[-(\frac{\sigma_x}{\epsilon_o \epsilon_n})\Delta t] \bigg] , \\ &+ \bigg[\frac{(\frac{\sigma_x}{\epsilon_o \epsilon_n})\Delta t}{(\frac{\sigma_x}{\epsilon_o \epsilon_n})\Delta t - (\gamma_\rho^{NL})\Delta t} \bigg] \bigg[\exp[-(\gamma_\rho^{NL})\Delta t] - \exp[-(\frac{\sigma_x}{\epsilon_o \epsilon_n})\Delta t] \bigg] , \\ &(\pi_{\rho,\delta}^{NL})_x &\equiv \int\limits_0^\Delta d\tau \int\limits_0^\tau d\tau' (\frac{\tau}{\Delta t}) \frac{(\tau',\tau')}{\Delta t} \cdot \exp[-(\gamma_\rho^{NL})\Delta t]^2] \bigg[\exp[-(\gamma_\rho^{NL})\Delta t] - \exp[-(\frac{\sigma_x}{\epsilon_o \epsilon_n})\Delta t] \bigg] , \\ &= (\Delta t)^2 \frac{\exp[(\frac{\sigma_x}{\epsilon_o \epsilon_n})\Delta t]}{[(\frac{\sigma_x}{\epsilon_o \epsilon_n})\Delta t]((\gamma_\rho^{NL})\Delta t)} \bigg\{ 1 - \frac{2}{(\frac{\sigma_x}{\epsilon_o \epsilon_n})\Delta t} - \frac{1}{(\gamma_\rho^{NL})\Delta t)} \bigg[- \frac{1}{(\gamma_\rho^{NL})\Delta t)} \bigg] \\ &+ \bigg[\frac{(\frac{\sigma_x}{\epsilon_o \epsilon_n})\Delta t}{[(\gamma_\rho^{NL})\Delta t)]((\frac{\sigma_x}{\epsilon_o \epsilon_n})\Delta t - (\gamma_\rho^{NL})\Delta t]} \bigg] \bigg[\exp[-(\gamma_\rho^{NL})\Delta t] - \exp[-(\frac{\sigma_x}{\epsilon_o \epsilon_n})\Delta t] \bigg] \bigg\} , \quad (A.124) \end{split}$$

$$\begin{split} (\pi_{\rho,7}^{NL})_x &\equiv \int\limits_0^{\Delta t} d\tau \int\limits_0^\tau d\tau' (\frac{\tau}{\Delta t})^2 \exp[-(\gamma_\rho^{NL})(\tau-\tau')] \exp[(\frac{\sigma_x}{\epsilon_0 \epsilon_R})\tau] \\ &= (\Delta t)^2 \frac{\exp[(\frac{\sigma_x}{\epsilon_0 \epsilon_R})\Delta t]}{[(\frac{\sigma_x}{\epsilon_0 \epsilon_R})\Delta t][(\gamma_\rho^{NL})\Delta t]} \left\{ 1 - \frac{3}{(\frac{\sigma_x}{\epsilon_0 \epsilon_R})\Delta t} + \frac{6}{(\frac{\sigma_x}{\epsilon_0 \epsilon_R})\Delta t]^2} - \frac{2}{(\gamma_\rho^{NL})\Delta t} + \frac{2}{[(\frac{\sigma_x}{\epsilon_0 \epsilon_R})\Delta t]^2} + \frac{4}{[(\gamma_\rho^{NL})\Delta t][(\frac{\sigma_x}{\epsilon_0 \epsilon_R})\Delta t]} - \left[1 - \exp[-(\frac{\sigma_x}{\epsilon_0 \epsilon_R})\Delta t] \right] \left[\frac{6}{[(\frac{\sigma_x}{\epsilon_0 \epsilon_R})\Delta t]^3} + \frac{4}{[(\gamma_\rho^{NL})\Delta t][(\frac{\sigma_x}{\epsilon_0 \epsilon_R})\Delta t]^2} - \frac{2}{[(\gamma_\rho^{NL})\Delta t]^2[(\frac{\sigma_x}{\epsilon_0 \epsilon_R})\Delta t]} \right] \\ &- \left[\frac{2[(\frac{\sigma_x}{\epsilon_0 \epsilon_R})\Delta t]}{[(\gamma_\rho^{NL})\Delta t][(\frac{\sigma_x}{\epsilon_0 \epsilon_R})\Delta t] - (\gamma_\rho^{NL})\Delta t} \right] \left[\exp[-(\gamma_\rho^{NL})\Delta t] - \exp[-(\frac{\sigma_x}{\epsilon_0 \epsilon_R})\Delta t] \right] \\ &+ \left[\frac{2[(\frac{\sigma_x}{\epsilon_0 \epsilon_R})\Delta t]}{[(\gamma_\rho^{NL})\Delta t][(\frac{\sigma_x}{\epsilon_0 \epsilon_R})\Delta t] - (\gamma_\rho^{NL})\Delta t} \right] \left[\exp[-(\gamma_\rho^{NL})\Delta t] - \exp[-(\frac{\sigma_x}{\epsilon_0 \epsilon_R})\Delta t] \right] \right\}, \quad (A.125) \end{split}$$

For the y component:

Replace $x \rightarrow y$ of matrix elements defined for the x component above.

For the z component:

Replace $x\rightarrow z$ of matrix elements defined for the x component above.

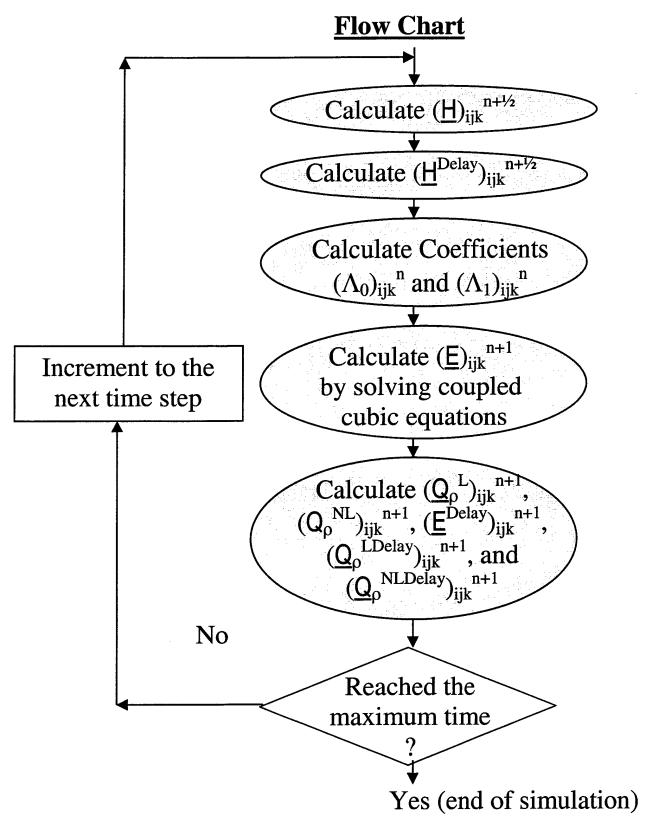


Figure 1: Flow chart of the nonlinear dispersive FDTD-PML algorithm

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